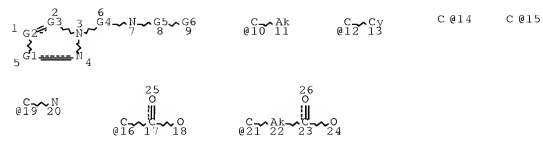
Case/Application number: 10/551,292
Priority Filing Date: 4/15/2003
Format for Search Results: Short
Meaning of Unusual Acronyms or Initialisms:

Identify the novelty:
    See limitation in amended claim 1 regarding X and 5A. "b molecule" may be searched open-ended.

Additional comments:
    Please search the structure in claim 1 amended 4/27/2009. See also specific structure in claim 24.

```
=> d que stat l7
L5                STR
```



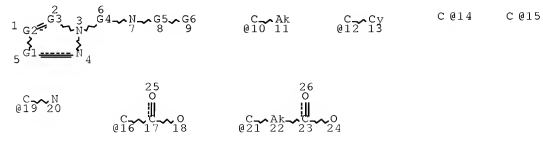
```
VAR G1=14/10/12
VAR G2=15/16/19/21
VAR G3=14/10/12
REP G4=(1-2) C
REP G5=(1-2) C
VAR G6=S/N/P
NODE ATTRIBUTES:
CONNECT IS E2  RC AT  14
CONNECT IS E2  RC AT  15
DEFAULT MLEVEL IS ATOM
GGCAT   IS UNS  AT  13
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  26

STEREO ATTRIBUTES: NONE
L7          827 SEA FILE=REGISTRY SSS FUL L5

100.0% PROCESSED  767106 ITERATIONS                          827 ANSWERS
SEARCH TIME: 00.01.01


=> d que stat l12
L5                STR
```

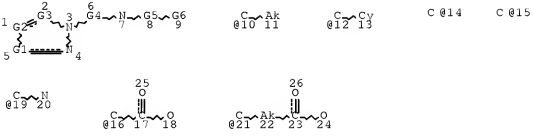


```
VAR G1=14/10/12
VAR G2=15/16/19/21
VAR G3=14/10/12
```

```
REP G4=(1-2) C
REP G5=(1-2) C
VAR G6=S/N/P
NODE ATTRIBUTES:
CONNECT IS E2  RC AT  14
CONNECT IS E2  RC AT  15
DEFAULT MLEVEL IS ATOM
GGCAT   IS UNS  AT  13
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  26

STEREO ATTRIBUTES: NONE
L7          827 SEA FILE=REGISTRY SSS FUL L5
L10             STR
```




```
VAR G1=14/10/12
VAR G2=15/16/19/21
VAR G3=14/10/12
REP G4=(1-2) CH2
REP G5=(1-2) CH2
VAR G6=S/N/P
NODE ATTRIBUTES:
CONNECT IS E1  RC AT  11
CONNECT IS E2  RC AT  14
CONNECT IS E2  RC AT  15
CONNECT IS E2  RC AT  22
DEFAULT MLEVEL IS ATOM
GGCAT   IS UNS  AT  13
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  26

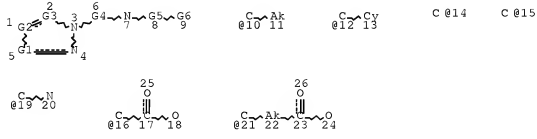
STEREO ATTRIBUTES: NONE
L12           90 SEA FILE=REGISTRY SUB=L7 SSS FUL L10

100.0% PROCESSED     827 ITERATIONS                          90 ANSWERS
SEARCH TIME: 00.00.01


=> d que nos 131
L5              STR
```

```
L7          827 SEA FILE=REGISTRY SSS FUL L5
L10             STR
L12          90 SEA FILE=REGISTRY SUB=L7 SSS FUL L10
L14             QUE  SPE=ON  ABB=ON  PLU=ON  SANTOS, I?/AU,AUTH
L15             QUE  SPE=ON  ABB=ON  PLU=ON  REGO, I?/AU,AUTH
L16             QUE  SPE=ON  ABB=ON  PLU=ON  CORREIA, J?/AU,AUTH
L17             QUE  SPE=ON  ABB=ON  PLU=ON  PAULO, A?/AU,AUTH
L18             QUE  SPE=ON  ABB=ON  PLU=ON  ALVES, S?/AU,AUTH
L19             QUE  SPE=ON  ABB=ON  PLU=ON  VITOR, R?/AU,AUTH
L20             QUE  SPE=ON  ABB=ON  PLU=ON  MALLINCKRODT/CS,SO,PA
L21             QUE  SPE=ON  ABB=ON  PLU=ON  AY<2004 OR PY<2004 OR PRY<20
                04 OR MY<2004 OR REVIEW/DT
L22             QUE  SPE=ON  ABB=ON  PLU=ON  BIOMOLECUL? OR (BIO(1W)MOLEC
                UL?) OR (BIOLOGIC?(3A)MOLECUL?)
L23             QUE  SPE=ON  ABB=ON  PLU=ON  CHELAT?
L24             QUE  SPE=ON  ABB=ON  PLU=ON  "CHELATING AGENTS"+PFT,OLD,N
                EW,NT/CT
L25          46 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L12
L26          19 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L25 AND (L22 OR L23
                OR L24)
L27          46 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  (L25 OR L26)
L28          18 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L27 AND (L14 OR L15
                OR L16 OR L17 OR L18 OR L19 OR L20)
L29          28 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L27 NOT L28
L30          23 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L29 AND L21
L31          28 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  (L29 OR L30)


=> d que stat l33
L10             STR
```




```
VAR G1=14/10/12
VAR G2=15/16/19/21
VAR G3=14/10/12
REP G4=(1-2) CH2
REP G5=(1-2) CH2
VAR G6=S/N/P
NODE ATTRIBUTES:
CONNECT IS E1  RC AT  11
CONNECT IS E2  RC AT  14
CONNECT IS E2  RC AT  15
CONNECT IS E2  RC AT  22
DEFAULT MLEVEL IS ATOM
GGCAT   IS UNS  AT  13
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
```

```
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  26

STEREO ATTRIBUTES: NONE
L33          10 SEA FILE=WPIX SSS FUL L10

100.0% PROCESSED   11053 ITERATIONS                          10 ANSWERS
SEARCH TIME: 00.00.13



=> d que nos l38
L10             STR
L14             QUE  SPE=ON  ABB=ON  PLU=ON  SANTOS, I?/AU,AUTH
L15             QUE  SPE=ON  ABB=ON  PLU=ON  REGO, I?/AU,AUTH
L16             QUE  SPE=ON  ABB=ON  PLU=ON  CORREIA, J?/AU,AUTH
L17             QUE  SPE=ON  ABB=ON  PLU=ON  PAULO, A?/AU,AUTH
L18             QUE  SPE=ON  ABB=ON  PLU=ON  ALVES, S?/AU,AUTH
L19             QUE  SPE=ON  ABB=ON  PLU=ON  VITOR, R?/AU,AUTH
L20             QUE  SPE=ON  ABB=ON  PLU=ON  MALLINCKRODT/CS,SO,PA
L22             QUE  SPE=ON  ABB=ON  PLU=ON  BIOMOLECUL? OR (BIO(1W)MOLEC
                UL?) OR (BIOLOGIC?(3A)MOLECUL?)
L23             QUE  SPE=ON  ABB=ON  PLU=ON  CHELAT?
L33          10 SEA FILE=WPIX SSS FUL L10
L34           3 SEA FILE=WPIX SPE=ON  ABB=ON  PLU=ON  (RABNX7/DCN OR RAFVJB/DCN
                 OR RAFVJC/DCN OR RAFVJD/DCN OR RAFVJE/DCN OR RAFVJF/DCN OR
                RAFVJG/DCN OR RAFVJ8/DCN OR RAFVJ9/DCN OR RAMT8E/DCN) OR
                L33/DCR
L35           2 SEA FILE=WPIX SPE=ON  ABB=ON  PLU=ON  L34 AND (L22 OR L23)
L36           3 SEA FILE=WPIX SPE=ON  ABB=ON  PLU=ON  (L34 OR L35)
L37           1 SEA FILE=WPIX SPE=ON  ABB=ON  PLU=ON  L36 AND (L14 OR L15 OR
                L16 OR L17 OR L18 OR L19 OR L20)
L38           2 SEA FILE=WPIX SPE=ON  ABB=ON  PLU=ON  L36 NOT L37


=> d que nos l39
L5              STR
L7          827 SEA FILE=REGISTRY SSS FUL L5
L10             STR
L12          90 SEA FILE=REGISTRY SUB=L7 SSS FUL L10
L39           0 SEA FILE=MEDLINE SPE=ON  ABB=ON  PLU=ON  L12


=> d que nos l41
L5              STR
L7          827 SEA FILE=REGISTRY SSS FUL L5
L10             STR
L12          90 SEA FILE=REGISTRY SUB=L7 SSS FUL L10
L41           0 SEA FILE=EMBASE SPE=ON  ABB=ON  PLU=ON  L12


=> d his l42

     (FILE 'BIOSIS, CABA, AGRICOLA, BIOTECHNO, DRUGU, VETU' ENTERED AT
     13:30:22 ON 25 JUN 2009)
L42           0 S L12

=> d que nos l42
L5              STR
L7          827 SEA FILE=REGISTRY SSS FUL L5
```

```
L10             STR
L12           90 SEA FILE=REGISTRY SUB=L7 SSS FUL L10
L42            0 SEA L12


=> dup rem l31 l38 l39 l41 l42
L39 HAS NO ANSWERS
L41 HAS NO ANSWERS
L42 HAS NO ANSWERS
FILE 'HCAPLUS' ENTERED AT 13:37:35 ON 25 JUN 2009
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE 'WPIX' ENTERED AT 13:37:35 ON 25 JUN 2009
COPYRIGHT (C) 2009 THOMSON REUTERS
PROCESSING COMPLETED FOR L31
PROCESSING COMPLETED FOR L38
PROCESSING COMPLETED FOR L39
PROCESSING COMPLETED FOR L41
PROCESSING COMPLETED FOR L42
L45           28 DUP REM L31 L38 L39 L41 L42 (2 DUPLICATES REMOVED)
                 ANSWERS '1-27' FROM FILE HCAPLUS
                 ANSWER '28' FROM FILE WPIX


=> file stnguide
FILE 'STNGUIDE' ENTERED AT 13:37:48 ON 25 JUN 2009
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FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Jun 19, 2009 (20090619/UP).

=> fil hcap wpix
FILE 'HCAPLUS' ENTERED AT 13:38:10 ON 25 JUN 2009
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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE 'WPIX' ENTERED AT 13:38:10 ON 25 JUN 2009
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=> d que l21
L21             QUE  SPE=ON  ABB=ON  PLU=ON  AY<2004 OR PY<2004 OR PRY<20
                04 OR MY<2004 OR REVIEW/DT


=> s l45 and l21
'2004' NOT A VALID FIELD CODE
'2004' NOT A VALID FIELD CODE
L46           23 L45 AND L21

=> dup rem l46
PROCESSING COMPLETED FOR L46
L47           23 DUP REM L46 (0 DUPLICATES REMOVED)
                 ANSWERS '1-22' FROM FILE HCAPLUS
                 ANSWER '23' FROM FILE WPIX

=> file stnguide
```

```
FILE 'STNGUIDE' ENTERED AT 13:39:14 ON 25 JUN 2009
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2009 AMERICAN CHEMICAL SOCIETY (ACS)

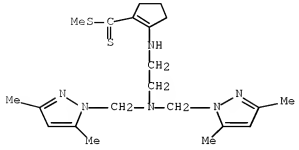
FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Jun 19, 2009 (20090619/UP).

=> d ibib ed abs hitind hitstr 1-22
YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS, WPIX' - CONTINUE? (Y)/N:y



L47  ANSWER 1 OF 23  HCAPLUS  COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER:         2000:862644  HCAPLUS  Full-text
DOCUMENT NUMBER:          134:246525
TITLE:                    Syntheses, structure and properties of cobalt-(II) and
                          -(III) complexes of pentadentate N4S ligands with
                          appended pyrazolyl groups: evidence for
                          cobalt(II)-dioxygen reversible binding
AUTHOR(S):                Bhattacharyya, Sudeep; Ghosh, Dipesh; Mukhopadhyay,
                          Suman; Jensen, William P.; Tiekink, Edward R. T.;
                          Chaudhury, Muktimoy
CORPORATE SOURCE:         Department of Inorganic Chemistry, Indian Association
                          for the Cultivation of Science, Calcutta, 700 032,
                          India
SOURCE:                   Dalton (2000), (24), 4677-4682
                          CODEN: DALTFG; ISSN: 1470-479X
PUBLISHER:                Royal Society of Chemistry
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
OTHER SOURCE(S):          CASREACT 134:246525
ED   Entered STN:  11 Dec 2000
AB   Cobalt-(II) and -(III) complexes of pentadentate N4S ligands based on Me 2-
     aminocyclopent-1-ene-1-carbodithioate with appended pyrazolyl groups (3,5-
     Me2C3HN2CH2)2NCH(R)CH2NHC5H6C(:S)SCH3 (R = H, Hmmecd; CH3, Hmmpcd) were
     prepared and characterized by IR, 1H NMR and electronic spectroscopy. Two of
     these compds. have also structurally been characterized by x-ray single
     crystal diffraction analyses.  Cobalt(II) in [Co(mmpcd)]ClO4 (1) shows a five-
     coordinate, trigonal bipyramidal geometry while its cobalt(III) counterpart,
     [Co(mmpcd)Cl]ClO4 (2), reveals a six-coordinated distorted octahedral
     structure by the inclusion of a chloride ligand in its equatorial plane.  In
     DMF or acetonitrile solution, 1 can bind dioxygen reversibly as indicated by
     EPR spectra recorded at cryogenic temps. Metal-dioxygen binding in 1 appears
     to be weak, possibly due to its trigonal bipyramidal structure and the
     presence of a sulfur donor in the ligand framework.  Electronic spectra of the
     cobalt(III) complexes show two LMCT bands in the near UV region, tentatively
     assigned to S→CoIII charge transfer.
CC   78-7 (Inorganic Chemicals and Reactions)
     Section cross-reference(s): 75, 77
IT   174280-57-0
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reactant for preparation of cobalt(III) Me
        (bis(dimethylpyrazolylmethyl)aminoethyl)aminocyclopentenecarbodithioato
        complex)
IT   174280-57-0
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reactant for preparation of cobalt(III) Me
        (bis(dimethylpyrazolylmethyl)aminoethyl)aminocyclopentenecarbodithioato
        complex)
```

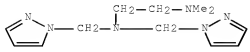
RN 174280-57-0 HCAPLUS
CN 1-Cyclopentene-1-carbodithioic acid, 2-[[2-[bis[(3,5-dimethyl-1H-pyrazol-1-yl)methyl]amino]ethyl]amino]-, methyl ester (CA INDEX NAME)



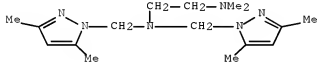
REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 2 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2001:43719 HCAPLUS Full-text
DOCUMENT NUMBER: 134:246535
TITLE: Cobalt(II) complexes of ethylenediamine-based pyrazole ligands: the crystal structure of [{N',N'-bis(3,5-dimethylpyrazol-1-ylmethyl)}-N,N-dimethylethylenediamine]cobalt(II) tetraphenylborate
AUTHOR(S): Lee, Soon Ae; Lim, Jong Wan; Roh, Soo-Gyun; Yeo, Hwan Jin; Jeong, Jong Hwa
CORPORATE SOURCE: Department of Chemistry, Kyungpook National University, Taegu, 702-701, S. Korea
SOURCE: Bulletin of the Korean Chemical Society (2000), 21(12), 1271-1273
CODEN: BKCSDE; ISSN: 0253-2964
PUBLISHER: Korean Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:246535
ED Entered STN: 18 Jan 2001
AB {N',N'-bis(pyrazol-1-ylmethyl)}-N,N-dimethylethylenediamine (L) and {N',N'-bis(3,5-dimethylpyrazol-1-ylmethyl)}-N,N-dimethylethylenediamine (L1) were prepared and complexed with CoCl2 to give [CoLCl]BPh4 and [CoL1Cl]BPh4. The crystal structure of [CoL1Cl]BPh40.5Me2CO was determined [crystal data: orthorhombic, space group P212121, Z = 8, R1 = 0.0617 , wR2 = 0.1488]. The complex has a trigonal bipyramidal structure in which Cl and 1 ethylenediamine N atom are axial.
CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 28, 75
IT 330153-74-7P 330153-75-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and complexation with cobalt)
IT 330153-74-7P 330153-75-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and complexation with cobalt)

RN 330153-74-7 HCAPLUS
CN 1,2-Ethanediamine, N1,N1-dimethyl-N2,N2-bis(1H-pyrazol-1-ylmethyl)- (CA INDEX NAME)



RN 330153-75-8 HCAPLUS
CN 1,2-Ethanediamine, N1,N1-bis[(3,5-dimethyl-1H-pyrazol-1-yl)methyl]-N2,N2-dimethyl- (CA INDEX NAME)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 3 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1999:687174 HCAPLUS Full-text
DOCUMENT NUMBER: 132:44035
TITLE: Palladium(II)-Induced Activation of Carbon-Nitrogen Single Bond of Coordinated N4S Ligand. Characterization of Product with Modified Ligand Structure: Kinetics versus Thermodynamic Considerations
AUTHOR(S): Bhattacharyya, Sudeep; Weakley, Timothy J. R.; Chaudhury, Muktimoy
CORPORATE SOURCE: Department of Inorganic Chemistry, Indian Association for the Cultivation of Science, Calcutta, 700 032, India
SOURCE: Inorganic Chemistry (1999), 38(23), 5453-5456
CODEN: INOCAJ; ISSN: 0020-1669
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 29 Oct 1999
AB Reaction of Pd(OAc)2 with 2-(β-bis(3,5-dimethylpyrazol-1-ylmethyl)aminoethylamino)cyclopent-1-enedithiocarboxylate (Hmmecd) in MeOH generated two products isolated as perchlorate salts, [Pd(N3S)-CH2Me2Pz]ClO4 (1) and [Pd(N3S)-CH2OMe]ClO4 (2). The square-planar mol. structure of 1 was determined by x-ray crystallog. Formation of 2 involves C-N bond cleavage and requires the presence of Pd(II). However, compound 1 once formed does not undergo methanolysis reaction further. Mechanistic implications of the C-N bond cleavage through a structural anomeric effect in an unstable reactive intermediate is discussed.
CC 78-7 (Inorganic Chemicals and Reactions)

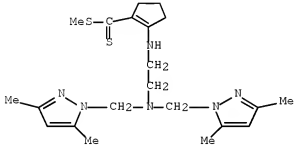
Section cross-reference(s): 67, 75

IT 67-56-1, Methanol, reactions 174280-57-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(palladium(II)-induced activation of carbon-nitrogen single bond of coordinated N4S ligand via methanolysis)

IT 174280-57-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(palladium(II)-induced activation of carbon-nitrogen single bond of coordinated N4S ligand via methanolysis)

RN 174280-57-0 HCAPLUS

CN 1-Cyclopentene-1-carbodithioic acid, 2-[[2-[bis[(3,5-dimethyl-1H-pyrazol-1-yl)methyl]amino]ethyl]amino]-, methyl ester (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 4 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1999:508196 HCAPLUS Full-text

DOCUMENT NUMBER: 131:214344

TITLE: Heterocyclic substituted silatranes. Part I. Synthesis and characterization of pyrazolyl substituted aminoalkylsilatranes

AUTHOR(S): Nasim, M.; Tharmaraj, P.; Venkataramani, P. S.

CORPORATE SOURCE: Defence Materials and Stores Research and Development Establishment DMSRDE PO, Kanpur, 208013, India

SOURCE: Synthesis and Reactivity in Inorganic and Metal-Organic Chemistry (1999), 29(7), 1249-1263
CODEN: SRIMCN; ISSN: 0094-5714

PUBLISHER: Marcel Dekker, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 16 Aug 1999

AB N-[Bis(3,5-dimethylpyrazol-1-ylmethyl)aminopropyl]- (6a) and N-[bis(3,5-dimethylpyrazol-1-ylmethyl)aminopropyl]-3,7,10- trimethylsilatranes (6b) were obtained in high yields from the reaction of N-[bis(3,5-dimethylpyrazol-1-ylmethyl)aminopropyl]triethoxysilane (3a) with triethanolamine (4a) or triisopropanolamine (4b). The corresponding N-Ph derivative (6c) was also obtained by the reaction of N-phenyl-[(3,5-dimethylpyrazol-1-ylmethyl)aminopropyl]trimethoxysilane (3b) with (4a). N-[3,5-Dimethylpyrazol-1-ylmethyl-3- silatranylaminopropyl]-N'-[bis(3,5-dimethylpyrazol-1-ylmethyl)]ethylenediamine (10a) and N-[3,5-dimethylpyrazol-1-ylmethyl]-3'-[(3,7,10- trimethylsilatranyl)aminopropyl]-N'-[bis(3,5-dimethylpyrazol-1-

ylmethyl)]ethylenediamine (10b) also were synthesized by the reaction of N-[3,5-dimethylpyrazol-1-ylmethyl]-N'-[bis(3,5-dimethylpyrazol-1-ylmethyl)ethylenediamine]trimethoxysilane (8) with (4a) and (4b). The precursor alkoxy compds. (3a), (3b) and (8) themselves were synthesized by reaction of 1-hydroxymethyl-3,5-dimethylpyrazole (2) with 3-aminopropyltriethoxy- (1a), N-phenylaminopropyltrimethoxy-(1b) and N-[2-aminoethyl(aminopropyl)]trimethoxysilanes (7), resp.

CC 29-6 (Organometallic and Organometalloidal Compounds)

IT 74789-21-2P 85952-93-8P 137684-04-9P 242464-71-7P 242464-72-8P 242464-74-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(for preparation of pyrazolyl substituted aminoalkylsilatranes)

IT 242464-66-0P 242464-67-1P 242464-68-2P 242464-69-3P 242464-70-6P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of pyrazolyl substituted aminoalkylsilatranes)

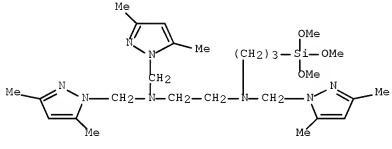
IT 242464-74-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(for preparation of pyrazolyl substituted aminoalkylsilatranes)

RN 242464-74-0 HCAPLUS

CN 1,2-Ethanediamine, N1,N1,N2-tris[(3,5-dimethyl-1H-pyrazol-1-yl)methyl]-N2-[3-(trimethoxysilyl)propyl]- (CA INDEX NAME)



IT 242464-69-3P 242464-70-6P

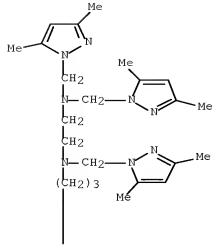
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of pyrazolyl substituted aminoalkylsilatranes)

RN 242464-69-3 HCAPLUS

CN 1,2-Ethanediamine, N1,N1,N2-tris[(3,5-dimethyl-1H-pyrazol-1-yl)methyl]-N2-[3-(2,8,9-trioxa-5-aza-1-silabicyclo[3.3.3]undec-1-yl)propyl]- (CA INDEX NAME)

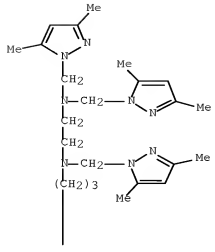
PAGE 1-A



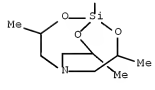
PAGE 2-A

RN 242464-70-6 HCAPLUS
CN 1,2-Ethanediamine, N1,N1,N2-tris[(3,5-dimethyl-1H-pyrazol-1-yl)methyl]-N2-[3-(3,7,10-trimethyl-2,8,9-trioxa-5-aza-1-silabicyclo[3.3.3]undec-1-yl)propyl]- (CA INDEX NAME)

PAGE 1-A

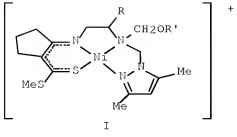


PAGE 2-A



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 5 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1999:65917 HCAPLUS Full-text
DOCUMENT NUMBER: 130:190922
TITLE: Nickel(II) in an N4S Donor Environment: An Unprecedented Alcoholysis Reaction through the Activation of a Carbon-Nitrogen Single Bond
AUTHOR(S): Bhattacharyya, Sudeep; Weakley, Timothy J. R.; Chaudhury, Muktimoy
CORPORATE SOURCE: Department of Inorganic Chemistry, Indian Association for the Cultivation of Science, Calcutta, 700 032, India
SOURCE: Inorganic Chemistry (1999), 38(4), 633-638
CODEN: INOCAJ; ISSN: 0020-1669
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 02 Feb 1999
GI



I

AB Pentadentate N4S ligands based on Me 2-aminocyclopent-1-ene-1-dithiocarboxylate with flexible pyrazolyl arms (Me2pzCH2)2NC2H3RNHC5H6CSSCH3 (R = H, Hmmecd and R = Me, Hmmpcd) undergo a nickel(II)-induced alcoholysis reaction through the activation of a saturated C-N bond linkage. The products obtained are square-planar complexes [(I); R = H, R' = Me (1); R = Me, R' = Me, Et, n-Pr (2-4)] containing a modified ligand structure possessing an N3S donor set and a pendant arm that holds the alkoxy group provided by the solvent. [Ni(N3S)-CH2OMe]ClO4 (1) crystallizes in the triclinic space group P.hivin.1 with a 10.4886(5), b 10.706(1), c 11.487(1) Å, α 108.784(4), β 108.887(6), γ 95.139(6)°, and Z = 2; while [Ni(N3S)'-CH2OPr]ClO4 (4) has the monoclinic space group P21/n with a 8.875(2), b 18.629(2), c 15.399(2) Å, β 91.37(2)°, and Z = 4 per unit cell. Complexes 1-4 with acyclic ligand environments have interesting electrochem. behavior in acetonitrile, involving a reversible Ni(II)/Ni(I) reduction, E1/2 .apprx.-1.0 V, and a Ni(II)/Ni(III) irreversible oxidation, Epa .apprx.1.0 V vs. Ag/AgCl as the reference The coulometrically reduced solution of 2 displays a rhombic EPR spectrum at 77 K characteristic of nickel(I) with g1 = 2.217, g2 = 2.170, and g3 = 2.054.

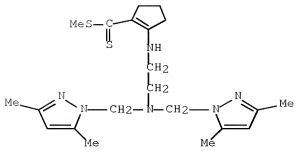
CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 72, 75

IT 64-17-5, Ethanol, reactions 67-56-1, Methanol, reactions 71-23-8, Propanol, reactions 174280-57-0 174280-58-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(nickel promoted alcoholysis of pyrazolylmethyl C-N bond in preparation of (pyrazolylmethylaminoalkyl)aminocyclopentenedithiocarboxylato complexes)

IT 174280-57-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(nickel promoted alcoholysis of pyrazolylmethyl C-N bond in preparation of (pyrazolylmethylaminoalkyl)aminocyclopentenedithiocarboxylato complexes)

RN 174280-57-0 HCAPLUS

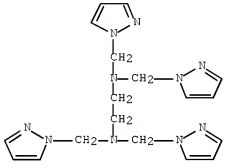
CN 1-Cyclopentene-1-carbodithioic acid, 2-[[2-[bis[(3,5-dimethyl-1H-pyrazol-1-yl)methyl]amino]ethyl]amino]-, methyl ester (CA INDEX NAME)



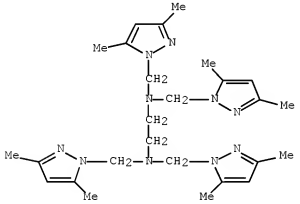
REFERENCE COUNT: 63 THERE ARE 63 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 6 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2000:237932 HCAPLUS Full-text
Correction of: 1997:64019
DOCUMENT NUMBER: 132:245490
Correction of: 126:219991
TITLE: Ion-pair extraction behavior of transition metal(II) cations as charged complexes with ethylenediamine derivatives having heterocyclic pendant arms
AUTHOR(S): Hirayama, Naoki; Iimuro, Shinji; Kubono, Koji; Kokusen, Hisao; Honjo, Takaharu
CORPORATE SOURCE: Kanazawa University, Kanazawa, 920-11, Japan
SOURCE: Analytica Chimica Acta (1997), 339(1-2), 115-121
CODEN: ACACAM; ISSN: 0003-2670
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 13 Apr 2000
AB The use of N,N,N',N'-tetrakis(1'-pyrazolylmethyl)-1,2-diaminoethane (tpzen), N,N,N',N'-tetrakis(3',5'-dimethylpyrazol-1'-ylmethyl)-1,2- diaminoethane (Me8tpzen) and N,N,N',N'-tetrakis(2'-pyridylmethyl)-1,2- diaminoethane (tpen) as complexation reagents for ion-pair extraction of metal(II) cations into nitrobenzene was studied. The order of extractability of the metals was tpen >> Me8tpzen > tpen. Although these mols. have four nitrogen-containing heterocyclic pendant arms and act as sexadentate ligands normally in aqueous solution, the result of numerical anal. concerning the extraction behavior indicated that they act as bidentate ligands in the extraction system. The pendant arms were not concerned in chelate formation and the arms acted to raise the hydrophobicity and the extractability of the complexes.
CC 79-4 (Inorganic Analytical Chemistry)
Section cross-reference(s): 68
IT 85264-42-2P 85264-43-3P
RL: ARG (Analytical reagent use); PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); PROC (Process); USES (Uses)
(preparation and dissociation constant and use in ion-pair extraction of transition metal(II) cations)
IT 85264-42-2P 85264-43-3P
RL: ARG (Analytical reagent use); PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); PROC (Process); USES (Uses)

(preparation and dissociation constant and use in ion-pair extraction of transition
metal(II) cations)
RN 85264-42-2 HCAPLUS
CN 1,2-Ethanediamine, N1,N1,N2,N2-tetrakis(1H-pyrazol-1-ylmethyl)- (CA INDEX NAME)

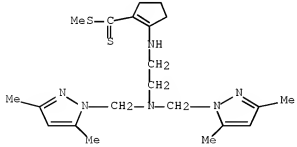


RN 85264-43-3 HCAPLUS
CN 1,2-Ethanediamine, N1,N1,N2,N2-tetrakis[(3,5-dimethyl-1H-pyrazol-1-yl)methyl]- (CA INDEX NAME)



L47 ANSWER 7 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1996:145239 HCAPLUS Full-text
DOCUMENT NUMBER: 124:218506
ORIGINAL REFERENCE NO.: 124:40069a,40072a
TITLE: Zinc(II) and Copper(II) Complexes of Pentacoordinating (N4S) ligands with Flexible Pyrazolyl Arms: Syntheses, Structure, Redox, and Spectroscopic Properties
AUTHOR(S): Bhattacharyya, Sudeep; Kumar, Sujit Baran; Dutta, Subodh Kanti; Tiekink, Edward R. T.; Chaudhury, Muktimoy
CORPORATE SOURCE: Department of Inorganic Chemistry, Indian Association for the Cultivation of Science, Calcutta, 700 032,

India
SOURCE: Inorganic Chemistry (1996), 35(7), 1967-73
CODEN: INOCAJ; ISSN: 0020-1669
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 124:218506
ED Entered STN: 13 Mar 1996
AB Zn(II) and Cu(II) complexes of two new potentially pentadentate ligands based on Me 2-aminocyclopent-1-ene-1-dithiocarboxylate with pendant pyrazolyl groups (pzCH2)2NC2H3RNHC5H6CSSCH3 (R = H, Hmmecd, and R = CH3, Hmmpcd, both having N4S donor atoms set) are reported. The mol. structures of [Zn(mmpcd)]ClO4 (1b) and [Cu(mmpcd)]ClO4 (2b) show a distorted trigonal bipyramidal geometry for the Zn(II) ion and a square pyramidal geometry for the Cu(II) ion. 1B crystallizes in the triclinic space group P.hivin.1, a 9.900(3), b 15.379(5), c 8.858(2) Å, α 99.93(2), β 93.62(2), γ 100.38(2)°, and Z = 2; while 2b crystallizes in the monoclinic space group P21/n, a 12.859(6), b 12.642(3), c 16.503(2) Å, β 102.67(2)°, and Z = 4. The structures were refined to final R = 0.042 for 1b and 0.049 for 2b. The EPR and electronic spectroscopic studies showed that the Cu(II) species doped into Zn(II) complex adopts the Zn(II) trigonal bipyramidal structure. The cyclic voltammetric measurements indicated 1-electron reversible reduction of the Cu(II) complex occurring at -0.74 V, while irreversible oxidation to Cu(III) takes place at +0.75 V (vs. Ag/AgNO3).
CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 72, 75
IT 174280-57-0P 174280-58-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and complexation with copper and zinc)
IT 174280-57-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and complexation with copper and zinc)
RN 174280-57-0 HCAPLUS
CN 1-Cyclopentene-1-carbodithioic acid, 2-[[2-[bis[(3,5-dimethyl-1H-pyrazol-1-yl)methyl]amino]ethyl]amino]-, methyl ester (CA INDEX NAME)



L47 ANSWER 8 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1996:358780 HCAPLUS Full-text
DOCUMENT NUMBER: 125:97176
ORIGINAL REFERENCE NO.: 125:18091a,18094a

TITLE: Formation of dinuclear copper(II) complex with N,N,N',N'-tetrakis(2-pyridylmethyl)-1,2-ethanediamine in aqueous solution

AUTHOR(S): Hirayama, Naoki; Iimuro, Shinji; Kubono, Koji; Kokusen, Hisao; Honjo, Takaharu

CORPORATE SOURCE: Dep. Chem., Kanazawa Univ., Kanazawa, 920-11, Japan

SOURCE: Talanta (1996), 43(4), 621-626
CODEN: TLNTA2; ISSN: 0039-9140

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 20 Jun 1996

AB The polynuclear complexation of divalent 3d transition metal cations with N,N,N',N'-tetrakis(2-pyridylmethyl)-1,2-ethanediamine (tpen) in aqueous solution was investigated. It was found that copper(II) forms a dinuclear complex with tpen in an aqueous solution containing chloride. The composition of the complex was determined as Cu2Cl2(tpen)2+. Furthermore, the stability constant of the structure was determined and its structure was postulated to be (μ-Cl)2.

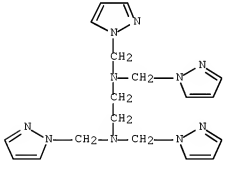
CC 68-3 (Phase Equilibriums, Chemical Equilibriums, and Solutions)

IT 7440-50-8D, Copper, (pyridyl)ethanediamine derivs. complexes 85264-42-2D, copper complexes 85264-43-3D, copper complexes
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(formation of copper(II) complexes with (pyridyl)ethanediamines)

IT 85264-42-2D, copper complexes 85264-43-3D, copper complexes
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(formation of copper(II) complexes with (pyridyl)ethanediamines)

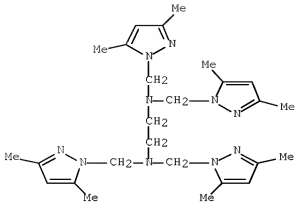
RN 85264-42-2 HCAPLUS

CN 1,2-Ethanediamine, N1,N1,N2,N2-tetrakis(1H-pyrazol-1-ylmethyl)- (CA INDEX NAME)



RN 85264-43-3 HCAPLUS

CN 1,2-Ethanediamine, N1,N1,N2,N2-tetrakis[(3,5-dimethyl-1H-pyrazol-1-yl)methyl]- (CA INDEX NAME)



L47 ANSWER 9 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1995:752087 HCAPLUS Full-text
DOCUMENT NUMBER: 123:186848
ORIGINAL REFERENCE NO.: 123:32901a,32904a
TITLE: Metal ion induced disintegration of a pyrazole-containing ligand and formation of an unprecedented pyrazolato-bridged di-zinc anion. The x-ray structure of the mixed ligand compound bis[(1,6-bis(3,5-dimethylpyrazol-1-yl)-2,5-dimethyl-2,5-diazahexane)(chlo ro)zinc(II)] [bis(μ-3,5-dimethylpyrazolato)tetrachlorodizincate(II)], [Zn(C16H28N6)Cl]2[Zn2(C5H7N2)2Cl4]
AUTHOR(S): Driessen, W. L.; Paap, F.; Reedijk, J.
CORPORATE SOURCE: Leiden Inst. Chemistry, Leiden Univ., Leiden, 2300 RA, Neth.
SOURCE: Recueil des Travaux Chimiques des Pays-Bas (1995), 114(7), 317-20
CODEN: RTCPA3; ISSN: 0165-0513
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 23 Aug 1995
AB The ligand 1,6-bis(3,5-dimethylpyrazol-1-yl)-2,5-dimethyl-2,5-diazahexane (debd), which was synthesized from 3,5-dimethylpyrazole, N,N'-dimethylethanediamine and formaldehyde, partially disintegrates when reacted with Zn dichloride or with Zn dibromide in MeOH. The resulting compds. contain the unique bis(pyrazolato)-bridged tetrahalo dizinc(II) anion. [Zn(debd)Cl]2[Zn2(dmpz)2Cl4], C42H70Cl6N16Zn4 and Mr = 1273.36, was obtained from MeOH as monoclinic crystals, space group P21/c with a 15.990(2), b 16.394(2), c 12.006(1) Å, β 100.61(1)°, V = 3093.4(5) Å3, Zm = 2, dc = 1.37 g cm-3, as measured at room temperature with Mo(Kα) radiation to a final R value of 0.062 (Rw = 0.065) for 2465 significant [I > 2σ(I)] reflections. The asym. unit comprises half the formula unit. The cation consists of a Zn2+ ion in a distorted trigonal bipyramidal environment of a chloride ion at 2.221(3) Å, an amine N at 2.17(1) Å and a pyrazole N at 2.05(1) Å in the equatorial plane, with an amine N at 2.27(1) and a pyrazole N at 2.14(1) Å in the axial positions. The largest distortion is in the axis of the trigonal bipyramid with an N-Zn-N angle of 150.2(5)°. The anion consists of two Zn2+ ions, which are bridged by two deprotonated dimethylpyrazole ligands with N-Zn distances

of 1.97(1) and 1.98(1) Å, while each Zn2+ ion is further bound to two chloride ions at 2.276(4) and 2.261(4) Å. The Zn2+ ions are in an almost regular N2Cl2 tetrahedron.

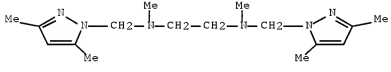
CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 75

IT 85264-39-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactions with zinc chloride and bromide)

IT 85264-39-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactions with zinc chloride and bromide)

RN 85264-39-7 HCAPLUS

CN 1,2-Ethanediamine, N1,N2-bis[(3,5-dimethyl-1H-pyrazol-1-yl)methyl]-N1,N2-dimethyl- (CA INDEX NAME)



L47 ANSWER 10 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1994:231747 HCAPLUS Full-text
DOCUMENT NUMBER: 120:231747
ORIGINAL REFERENCE NO.: 120:40821a,40824a
TITLE: Processing of silver halide color photographic material for stable images
INVENTOR(S): Fujita, Yoshihiro; Nakamura, Shigeru
PATENT ASSIGNEE(S): Fuji Photo Film Co Ltd, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 194 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05034888	A	19930212	JP 1991-214219	19910801 <--
PRIORITY APPLN. INFO.:			JP 1991-214219	19910801 <--

ED Entered STN: 30 Apr 1994

GI For diagram(s), see printed CA Issue.

AB Ag halide color photog. material containing yellow coupler I(R1 = tertiary alkyl or aryl; R2 = H, halo, alkoxy, aryloxy, alkyl, dialkylamino; R3 = substituent; X = heterocyclyl bonded to the coupling active position through aryloxy or N, and releasable on coupling reaction with oxidized aromatic primary amine developer; a = 0-4; R3 may be same or different when a ≥ 2) is processed by employing a processing solution containing II or III(X = nonmetallic atoms required to form 4-8-membered ring; atoms bonded to N are selected from C, O, S; X0 = nonmetallic atoms required to form N-containing heterocycle; Ra, Rb = alkyl, alkenyl, or bonded to each other to form a 4-8-

membered ring). The processing improved yellow image fastness leading to improved image storage stability.

IC ICM G03C011-00
ICS G03C007-36

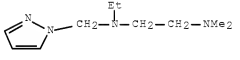
CC 74-2 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

IT 288-13-1, 1H-Pyrazole 288-88-0, 1H-1,2,4-Triazole 76686-85-6
91272-91-2 91272-92-3 144986-76-5 149310-10-1 150704-12-4
RL: USES (Uses)
(yellow image stabilizer, processing solution containing)

IT 150704-12-4
RL: USES (Uses)
(yellow image stabilizer, processing solution containing)

RN 150704-12-4 HCAPLUS

CN 1,2-Ethanediamine, N1-ethyl-N2,N2-dimethyl-N1-(1H-pyrazol-1-ylmethyl)- (CA INDEX NAME)



L47 ANSWER 11 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1994:123377 HCAPLUS Full-text

DOCUMENT NUMBER: 120:123377

ORIGINAL REFERENCE NO.: 120:21521a,21524a

TITLE: Copper(II) coordination chemistry of potentially octadentate (N8) tetrapyridyl and tetrapyrazolyl-pyridazine ligands. X-ray crystal structures of [Cu2(PTAPY)Br4]·2DMF and [Cu2(PTAPY)(NO3)2(N3)(H2O)]2(NO3)2·1.2CH3OH

AUTHOR(S): Tandon, Santokh S.; Chen, Liqin; Thompson, Laurence K.; Connors, Sean P.; Bridson, John N.

CORPORATE SOURCE: Department of Chemistry, Memorial University of Newfoundland, St. John's, Nfld., A1B 3X7, Can.

SOURCE: Inorganica Chimica Acta (1993), 213(1-2), 289-300
CODEN: ICHAA3; ISSN: 0020-1693

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 05 Mar 1994

AB The structural, electrochem., ESR and magnetic properties of dinuclear Cu(II) complexes of 2 new polyfunctional pyridazine ligands, 3,6-bis(N,N,N',N'-tetrakis(pyridin-2- ylmethyl)aminoethanethiolato)pyridazine (PTAPY), and 3,6-bis(N,N,N',N'-tetrakis(pyrazol-1- ylmethyl)aminoethanethiolato)pyridazine (PTAPZ) are discussed. PTAPY and PTAPZ are potentially octadentate (N8) ligands and on reaction with Cu(II)salts form dinuclear complexes, [Cu2(PTAPY)X4].yH2O (X = NO3, y = 1; X = Br, y = 2), [Cu2(PTAPY)(MeCN)2](ClO4)4.0.5EtOH, [Cu2(PTAPZ)Cl4].5H2O, and tetranuclear [Cu2(PTAPY)(NO3)2(N3)(H2O)]2(NO3)2.1.2CH3OH (I). The single crystal x-ray structures of [Cu2(PTAPY)Br4].2DMF (II) and I were determined, and in each case the ligand is hexadentate. Two different 5-coordinate (CuN3Br2) geometries exist within II. In I, the 2 Cu atoms are quite different with 6-(axially elongated, distorted tetragonal) and 5- (distorted square-pyramidal) coordinate arrangements, and dimerization through azido N atoms gave a

tetranuclear N3- bridged mol. The pyridazine N atoms remain uncoordinated in all complexes and there is no magnetic interaction between the distant Cu centers. Cyclic voltammograms are characterized by the presence of either 1 2-electron or 2 1-electron (overlapping) reversible or quasi-reversible redox processes, associated with the reduction of the dinuclear Cu(II) species to dinuclear Cu(I) species.

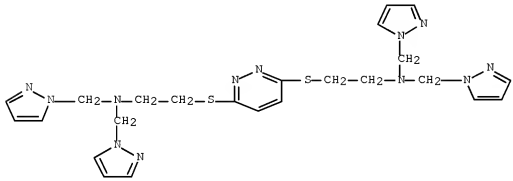
CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 28, 75

IT 152305-82-3P 152305-83-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with copper salts)

IT 152305-83-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with copper salts)

RN 152305-83-4 HCAPLUS

CN 1H-Pyrazole-1-methanamine, N,N'-[3,6-pyridazinediylbis(thio-2,1-ethanediyl)]bis[N-(1H-pyrazol-1-ylmethyl)- (9CI) (CA INDEX NAME)



L47 ANSWER 12 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER:	1993:613909 HCAPLUS Full-text
DOCUMENT NUMBER:	119:213909
ORIGINAL REFERENCE NO.:	119:37907a,37910a
TITLE:	Method for processing color photographic material
INVENTOR(S):	Fujimoto, Hiroshi; Fujita, Yoshihiro; Nakamura, Shigeru
PATENT ASSIGNEE(S):	Fuji Photo Film Co., Ltd., Japan
SOURCE:	Jpn. Kokai Tokkyo Koho, 89 pp. CODEN: JKXXAF
DOCUMENT TYPE:	Patent
LANGUAGE:	Japanese
FAMILY ACC. NUM. COUNT:	1
PATENT INFORMATION:	

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04362945	A	19921215	JP 1991-193593	19910709 <--
PRIORITY APPLN. INFO.:			JP 1991-99721	A1 19910405 <--

ED Entered STN: 13 Nov 1993

GI For diagram(s), see printed CA Issue.

AB In the title processing method, the color photog. material contains ≥1 high b.p. organic solvent described by O:P(OR1)(OR2)(OR3) and I [R1-5 = alkyl, cycloalkyl, aryl; R6 = halo, alkyl, alkoxy, aryloxy, alkoxycarbonyl; a = 0-3] in its red- and/or green-sensitive photog. emulsion layers, and is processed with a solution containing II and/or III [X = non-metallic atoms required to complete a 4- to 8-membered ring; only C, O, and S can bond to N; X0 = non-metallic atoms required to complete a N-containing hetero-aromatic ring; R7,8 = alkyl, alkenyl; R7 and R8 may form a 4- to 8-membered ring] after being color developed. This method improves stability of magenta dye images.

IC ICM G03C011-00
ICS G03C001-38; G03C007-388; G03C007-42

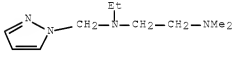
CC 74-2 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 41

IT 951-49-5 78758-54-0 91272-92-3 98816-32-1 144986-84-5
144986-86-7 146456-97-5 146475-24-3 149310-08-7 150704-05-5
150704-06-6 150704-07-7, 1H-Pyrazole-1,4-dimethanol 150704-08-8
150704-09-9 150704-10-2 150704-11-3 150704-12-4
150704-13-5 150704-14-6 150704-15-7 150704-16-8
RL: USES (Uses)
(photog. stabilizer containing)

IT 150704-12-4
RL: USES (Uses)
(photog. stabilizer containing)

RN 150704-12-4 HCAPLUS

CN 1,2-Ethanediamine, N1-ethyl-N2,N2-dimethyl-N1-(1H-pyrazol-1-ylmethyl)- (CA INDEX NAME)



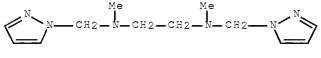
L47 ANSWER 13 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1993:29868 HCAPLUS Full-text
DOCUMENT NUMBER: 118:29868
ORIGINAL REFERENCE NO.: 118:5361a,5364a
TITLE: Processing solution for silver halide color photographic material
INVENTOR(S): Morigaki, Masakazu; Kawamoto, Hiroyuki; Nakamura, Shigeru
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Eur. Pat. Appl., 113 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 504609	A2	19920923	EP 1992-102855	19920220 <--
EP 504609	A3	19930303		
EP 504609	B1	19950719		

R: BE, DE, GB

JP 04313753	A	19921105	JP 1991-142708	19910520 <--
JP 2729542	B2	19980318		
US 5449593	A	19950912	US 1992-838963	19920221 <--
US 5576151	A	19961119	US 1995-426671	19950421 <--
PRIORITY APPLN. INFO.:			JP 1991-48679 A	19910222 <--
			JP 1991-142708 A	19910520 <--
			US 1992-838963 A3	19920221 <--

OTHER SOURCE(S): MARPAT 118:29868
ED Entered STN: 24 Jan 1993
GI For diagram(s), see printed CA Issue.
AB A solution for processing a Ag halide color photog. material for producing color images having excellent storage stability contains ≥1 compound selected from compds. represented by formulas I, II, and III (Z1 = a nonmetallic atomic group bonding to each N atom with a C, O, or S atom to form a 4- to 8-membered ring; R1, R2 = H, alkyl, alkenyl, aryl, acyl, sulfonyl, sulfinyl, hydroxy, acyloxy, acylamino, sulfonamido, ureido, sulfamoylamino, alkoxycarbonylamino, carbamoyl, sulfamoyl, or heterocyclyl; X1-4 = NR4, N, O, S, CR5R6, CR5, CO, or CNR7 where R4-7 or a substituent group; Z2-4 = a nonmetallic atomic group necessary for forming a 4- to 8-membered ring; Y = O or S; R3 = alkyl, alkenyl, aryl, acyl, sulfonyl, sulfinyl, alkoxycarbonyl, carbamoyl, sulfamoyl, oxalyl, or heterocyclyl).
IC ICM G03C007-30
ICS G03C007-407; G03C007-42
CC 74-2 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
IT 23230-43-5 67685-12-5 75663-96-6 85264-38-6 91272-74-1
91272-91-2 91272-92-3 93597-03-6 101213-03-0 144986-76-5
144986-77-6 144986-78-7 144986-79-8 144986-80-1 144986-81-2
144986-82-3 144986-83-4 144986-84-5 144986-85-6 144986-86-7
144986-87-8 144986-88-9 144986-89-0 144986-90-3 144986-91-4
RL: USES (Uses)
(color photog. stabilizing solns. containing)
IT 85264-38-6
RL: USES (Uses)
(color photog. stabilizing solns. containing)
RN 85264-38-6 HCAPLUS
CN 1,2-Ethanediamine, N1,N2-dimethyl-N1,N2-bis(1H-pyrazol-1-ylmethyl)- (CA INDEX NAME)



L47 ANSWER 14 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1992:206551 HCAPLUS Full-text
DOCUMENT NUMBER: 116:206551
ORIGINAL REFERENCE NO.: 116:34763a,34766a
TITLE: Transition metal complexes of two related pyrazole containing ligands: 3,6-dimethyl-1,8-bis(3,5-dimethyl-1-pyrazolyl)-3,6-diazaoctane (ddad) and 1,4-bis(2-(3,5-dimethyl-1-pyrazolyl)ethyl)piperazine (bedp). Synthesis, spectroscopy and x-ray structures

AUTHOR(S): Haanstra, W. G.; Driessen, W. L.; De Graaff, R. A. G.; Sebregts, G. C.; Suriano, J.; Reedijk, J.; Turpeinen, U.; Hamalainen, R.; Wood, J. S.

CORPORATE SOURCE: Dep. Chem., Leiden Univ., Leiden, 2300 RA, Neth.

SOURCE: Inorganica Chimica Acta (1991), 189(2), 243-51
CODEN: ICHAA3; ISSN: 0020-1693

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 16 May 1992

AB Several coordination compds. with 3,6-dimethyl-1,8-bis(3,5-dimethyl-1-pyrazolyl)-3,6-diazaoctane (ddad) were obtained: [M(ddad)](BF4)2 (I; M = Cu, Ni), Co(ddad)(H2O)(BF4)2, M2(ddad)Cl4 (II; M = Co, Ni, Cu, Zn), Co3(ddad)2(NCS)6 (III) and Cu2(ddad)(NCS)3 (IV). Five x-ray structures were obtained, viz. of I, Ni(ddad)(NCS)2 (V), [Ni(bedp)](H2O)(BF4)2 (bedp = 3,6-dimethyl-1,8-bis(3,5-dimethyl-1-pyrazolyl)-3,6-diazaoctane) and [Cu(bedp)](H2O)(BF4)2, but the data did not allow the calcn. of very accurate bond lengths. However, the basic coordination geometries were obtained in all cases. The coordination by the ligands is square planar, while V contains addnl. trans coordinating thiocyanate anions. The asym. unit of I (M = Cu) contains two almost identical [Cu(ddad)]2+ species. The coordination of the copper atoms in both mols. is intermediate between tetrahedral and square planar. [Cu(ddad)]2+ exists as the (R,R) and (S,S) diastereoisomers of the ligand. II are, except for M = Ni), all dinuclear with MN2Cl2 chromophores. II (M = Ni) contains square planar Ni(ddad)2+ cations and tetrahedral NiCl42- anions. V, which is isomorphous with the corresponding Zn(II) compds., has octahedral MN2N2'N2'' chromophores. III crystallizes as [Co(ddad)(NCS)]2Co(NCS)4 with five coordinate cobalt in the cation. IV is formulated as [Cu(ddad)]2+ and [Cu(NCS)3]2-. [M(bedp)](H2O)(BF4)2(M = Ni, Cu), M(bedp)(NCS)2 (M = Ni, Co), Zn2(bedp)(NCS)4, M2(bedp)Cl4 (VI; M = Ni, Co, Cu, Zn) and Cu2(bedp)(NCS)3 (VII) were obtained. VI form dinuclear compds. (similar to ddad) with MN2Cl2 chromophores. However, in addition to the green form of [Ni(bedp)][NiCl4] a purple isomer Ni2(bedp)Cl4, with a tetrahedral NiN2Cl2 chromophore, was obtained. The ligand field spectra of V and the isomorphous cobalt compound show typical octahedral chromophores. VII has a structure likely to be similar to the corresponding ddad compound, viz. [Cu(II)(bedp)][Cu(I)(SCN)3]. The prepns. of the ligands are described.

CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 28, 75

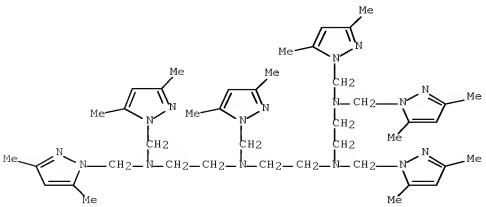
IT 139775-87-4P 139775-88-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and complexation of)

IT 139775-87-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and complexation of)

RN 139775-87-4 HCAPLUS

CN 1,2-Ethanediamine, N1,N2-bis[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]-N1,N2-dimethyl- (CA INDEX NAME)

L47 ANSWER 15 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1989:184768 HCAPLUS Full-text
DOCUMENT NUMBER: 110:184768
ORIGINAL REFERENCE NO.: 110:30457a,30460a
TITLE: Dinuclear transition metal compounds of a decadentate pyrazole-containing chelating ligand. X-ray crystal structure of Co2(tthd)(ClO4)4(H2O)2(MeOH)1.75
AUTHOR(S): Paap, F.; Driessen, W. L.; De Graaff, R. A. G.; Reedijk, J.
CORPORATE SOURCE: Dep. Chem., Leiden Univ., Leiden, 2300 RA, Neth.
SOURCE: Polyhedron (1988), 7(24), 2575-81
CODEN: PLYHDE; ISSN: 0277-5387
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 12 May 1989
AB A potentially decadentate ligand, 1,1,4,7,10,10-hexakis(3,5-dimethyl-1-pyrazolylmethyl)-1,4,7,10-tetraazadecane (H2tthd), was prepared from the reaction of triethylenetetramine with 6 equiv of N-hydroxymethyl-3,5-dimethylpyrazole. M2(tthd)(ClO4)4(H2O)x (M = Co, Ni, Cu, Zn, Cd; x = 4-8) and M2(tthd)X2(ClO4)2(H2O)x (M = Co, Ni; X = NCS, Cl; x = 4-8) were prepared Co2(tthd)(ClO4)4(H2O)2(MeOH)1.75 crystallizes in the triclinic space group P1, a 1.959(2), b 1.5657(3), c 2.1244(3) nm, α 105.5(1), β 96.9(1), γ 112.1(1)°. Due to severe disorder of the anions the structure could only be refined to Rw = 0.099. The ligand acts as a decadentate, dinucleating ligand. The Co ions are distorted octahedrally, surrounded by 5 N-atoms of the tthd ligand and an O atom of water occupying the 6th coordination place. The other perchlorate compds. have very similar structures, as can be concluded from spectroscopic data. In the thiocyanate and chloride compds. the anions replace coordinated H2O mols., resulting in octahedral Ni compds. With Co thiocyanate, however, tthd acts as an octadentate ligand, resulting only in 5-coordinated compds.
CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 28, 75
IT 85264-45-5P 119781-62-3P 120170-22-1P 120170-25-4P 120170-28-7P 120183-41-7P 120183-44-0P 120293-21-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 85264-45-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 85264-45-5 HCAPLUS
CN 1,2-Ethanediamine, N1,N2-bis[2-[bis[(3,5-dimethyl-1H-pyrazol-1-yl)methyl]amino]ethyl]-N1,N2-bis[(3,5-dimethyl-1H-pyrazol-1-yl)methyl]- (CA INDEX NAME)



L47 ANSWER 16 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1989:185371 HCAPLUS Full-text
DOCUMENT NUMBER: 110:185371
ORIGINAL REFERENCE NO.: 110:30551a,30554a
TITLE: 3,5-Diphenyl-1H-pyrazole derivatives. II. N-Substituted 1-(2-aminoethyl)-3,5-diphenyl-1H-pyrazoles and their 4-bromo derivatives with analgesic and other activities
AUTHOR(S): Bondavalli, F.; Bruno, O.; Ranise, A.; Schenone, P.; Russo, S.; Loffreda, A.; De Novellis, V.; Lo Sasso, C.; Marmo, E.
CORPORATE SOURCE: Ist. Sci. Farm., Univ. Genova, Genoa, Italy
SOURCE: Farmaco, Edizione Scientifica (1988), 43(12), 1019-34
CODEN: FRPSAX; ISSN: 0430-0920
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 110:185371
ED Entered STN: 26 May 1989
GI

I

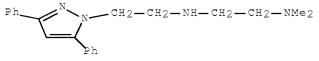
AB Eighteen title compds. (I, R = H, alkyl; R1 = alkyl; RR1 = alkylene, alkyleneoxyalkylene, alkyleneiminoalkylene, and etc.; R2 = H, Br) were prepared by reaction of the corresponding 1-(2-hydroxyethyl) compds. with tosyl chloride, followed by refluxing the resultant tosylates with an excess of primary or secondary amine. I had marked analgesic activity. Moreover, various I had moderate hypotensive, bradycardic, anti-inflammatory, and local anesthetic activity in vivo, as well as weak platelet-antiaggregating potency in vitro.

CC 1-4 (Pharmacology)
Section cross-reference(s): 28

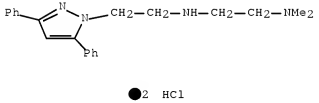
IT 4162-98-5P 120217-55-2P 120217-56-3P 120217-57-4P
120217-58-5P 120217-59-6P 120217-60-9P 120217-61-0P 120217-62-1P
120217-63-2P 120217-64-3P 120217-65-4P 120217-66-5P 120217-67-6P
120217-68-7P 120217-69-8DP, derivs. 120217-72-3P 120217-73-4P
120217-74-5P 120217-75-6P 120217-76-7P 120217-77-8P 120217-78-9P
120217-79-0P 120217-80-3P 120217-81-4P 120217-82-5P 120217-83-6P
120253-58-9P 120253-59-0P 120253-60-3P
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(preparation and pharmacol. of)

IT 120217-57-4P 120217-73-4P
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic

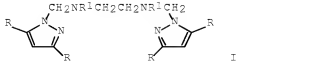
preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(preparation and pharmacol. of)
RN 120217-57-4 HCAPLUS
CN 1,2-Ethanediamine, N'-[2-(3,5-diphenyl-1H-pyrazol-1-yl)ethyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)



RN 120217-73-4 HCAPLUS
CN 1,2-Ethanediamine, N'-[2-(3,5-diphenyl-1H-pyrazol-1-yl)ethyl]-N,N-dimethyl-, dihydrochloride (9CI) (CA INDEX NAME)



L47 ANSWER 17 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1988:197156 HCAPLUS Full-text
DOCUMENT NUMBER: 108:197156
ORIGINAL REFERENCE NO.: 108:32217a,32220a
TITLE: Copper complexes of some tetradentate pyrazolyl amines
AUTHOR(S): Addison, A. W.; Palaniandavar, M.; Driessen, W. L.; Paap, F.; Reedijk, J.
CORPORATE SOURCE: Chem. Dep., Drexel Univ., Philadelphia, PA, 19104, USA
SOURCE: Inorganica Chimica Acta (1988), 142(1), 95-100
CODEN: ICHAA3; ISSN: 0020-1693
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 28 May 1988
GI



AB I [R = R1 = H (edbp); R = Me, R1 = H (edbd); R = H, R1 = Me (debp); R = R1 = Me (debd)] were prepared by condensation of N-hydroxymethylpyrazoles with ethylenediamines. CuL(ClO4)2 (L = debp, edbp, edbd) and Cu(debd)(dMp)X2 (X = ClO4, BF4; dMp = 3,5-dimethylpyrazole) were prepared The compds. were characterized by their absorption (d-d) and EPR spectra. All 4 undergo quasi-reversible electrochem. reduction in MeOH, the redox potentials being correlated with the degree of ligand methylation. The Cu(I) complexes are relatively unstable and bind CO with different affinities.

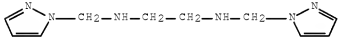
CC 78-7 (Inorganic Chemicals and Reactions)

IT 114287-01-3P 114315-22-9P 114315-23-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 114315-22-9P 114315-23-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

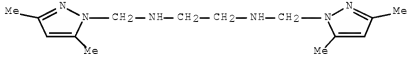
RN 114315-22-9 HCAPLUS

CN 1,2-Ethanediamine, N1,N2-bis(1H-pyrazol-1-ylmethyl)- (CA INDEX NAME)



RN 114315-23-0 HCAPLUS

CN 1,2-Ethanediamine, N1,N2-bis[(3,5-dimethyl-1H-pyrazol-1-yl)methyl]- (CA INDEX NAME)



L47 ANSWER 18 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1989:106933 HCAPLUS Full-text

DOCUMENT NUMBER: 110:106933

ORIGINAL REFERENCE NO.: 110:17483a,17486a

TITLE: Transition metal complexes of ligands containing 3,5-dimethylpyrazolyl groups and thioether functions. The crystal and molecular structure of (1,12-bis(3,5-dimethylpyrazol-1-yl)-2,11-diaza-5,8-dithiadodecane)nickel(II) bis(tetrafluoroborate)

AUTHOR(S): Paap, F.; Driessen, W. L.; Reedijk, J.; Spek, A. L.

CORPORATE SOURCE: Dep. Chem., Leiden Univ., Leiden, 2300 RA, Neth.

SOURCE: Inorganica Chimica Acta (1988), 150(1), 57-64
CODEN: ICHAA3; ISSN: 0020-1693

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 17 Mar 1989

AB The hexadentate (N4S2) ligand 1,12-bis(3,5-dimethylpyrazol-1-yl)-2,11- diaza-5,8-dithiadodecane (dsbd) forms M(dsbd)A2 (M = Co, Ni or Cd; A = ClO4 or BF4).

Ni(dsbd)(BF4)2 crystallizes in the monoclinic space group P21/n, Z = 4, a 1.2817(4), b 1.5512(3), c 1.33666(4) nm, β 94.11(1)°, Rw = 0.032 for 2181 observed reflections. The Ni ion is octahedrally chelated by 2 S atoms, 2 amine nitrogens and 2 pyrazole nitrogens. Ni-N amts. to 210-212 pm, Ni-S distances are 243.5 pm. The other dsbd compds. have very similar structures as is concluded from their spectroscopic properties. The octadentate (N6S2) ligand 1,1,10,10-tetrakis(3,5-dimethylpyrazol-1-ylmethyl)-1,10-diaza-4,7-dithiadecane (dstd) forms M2(dstd)A4(H2O)n, (M = Mn, Fe, Co, Ni, Cu, Zn or Cd; A = ClO4, n = 4; M = Co, Ni or Zn, A = BF4, n = 4; M = Co or Ni, A = NCS, n = 0). In all compds. the metal ions are 6-coordinated, as deduced from their spectroscopic properties.

CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 75

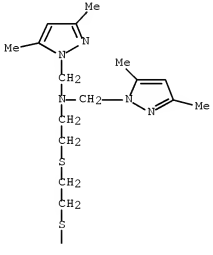
IT 118202-79-2P, 1,1,10,10-Tetrakis(3,5-dimethylpyrazol-1-ylmethyl)-1,10-diaza-4,7-dithiadecane 118202-80-5P, 1,12-Bis(3,5-dimethylpyrazol-1-yl)-2,11-diaza-5,8-dithiadodecane 118473-35-1P 118473-36-2P 118473-38-4P 118473-39-5P 118473-42-0P 118473-43-1P 118473-45-3P 118504-38-4P 118504-40-8P 118504-41-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 118202-79-2P, 1,1,10,10-Tetrakis(3,5-dimethylpyrazol-1-ylmethyl)-1,10-diaza-4,7-dithiadecane 118202-80-5P, 1,12-Bis(3,5-dimethylpyrazol-1-yl)-2,11-diaza-5,8-dithiadodecane
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

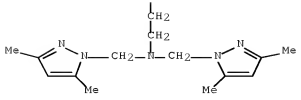
RN 118202-79-2 HCAPLUS

CN 1H-Pyrazole-1-methanamine, N,N'-[1,2-ethanediylbis(thio-2,1-ethanediyl)]bis[N-[(3,5-dimethyl-1H-pyrazol-1-yl)methyl]-3,5-dimethyl- (9CI) (CA INDEX NAME)

PAGE 1-A

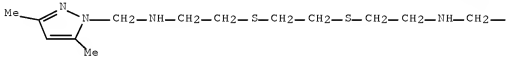


PAGE 2-A

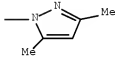


RN 118202-80-5 HCAPLUS
CN 1H-Pyrazole-1-methanamine, N,N'-[1,2-ethanediylbis(thio-2,1-ethanediyl)]bis[3,5-dimethyl- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



L47 ANSWER 19 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1987:94880 HCAPLUS Full-text
DOCUMENT NUMBER: 106:94880
ORIGINAL REFERENCE NO.: 106:15371a,15374a
TITLE: Five- and six-coordinated transition-metal mixed-anion compounds containing the sterically constrained pyrazole-containing ligand 1,6-bis(3',5'-dimethylpyrazol-1'-yl)-2,5-dimethyl-2,5-diazahexane
AUTHOR(S): Paap, Frans; Driessen, Willem L.; Reedijk, Jan
CORPORATE SOURCE: Dep. Chem., State Univ. Leiden, Leiden, 2300 RA, Neth.
SOURCE: Polyhedron (1986), 5(11), 1815-19
CODEN: PLYHDE; ISSN: 0277-5387
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 21 Mar 1987
AB The dimethylpyrazole derivative of N,N-dimethylethylenediamine, viz. 1,6-bis(3',5'-dimethylpyrazol-1'-yl)-2,5-diazahexane (debd), forms coordination compds. with the transition-metal ions (M = Co(II), Ni(II), Cu(II) and Zn(II)) in the presence of a halide and a ClO4--anion of stoichiometry [M(debd)X(H2O)n]ClO4 (n = 0 or 1). The ligand is always tetradentate. With Co and Ni 6-coordinate compds. are formed. With Cu and Zn 5-coordinate

compds. are formed. The compds. were characterized by spectroscopic and magnetic methods (IR, ligand field, ESR and NMR).

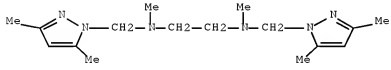
CC 78-7 (Inorganic Chemicals and Reactions)

IT 85264-39-7, 1,6-Bis(3,5-dimethylpyrazol-1-yl)-2,5-dimethyl-2,5-diazahexane
RL: PRP (Properties)
(NMR of)

IT 85264-39-7, 1,6-Bis(3,5-dimethylpyrazol-1-yl)-2,5-dimethyl-2,5-diazahexane
RL: PRP (Properties)
(NMR of)

RN 85264-39-7 HCAPLUS

CN 1,2-Ethanediamine, N1,N2-bis[(3,5-dimethyl-1H-pyrazol-1-yl)methyl]-N1,N2-dimethyl- (CA INDEX NAME)



L47 ANSWER 20 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1986:140923 HCAPLUS Full-text

DOCUMENT NUMBER: 104:140923

ORIGINAL REFERENCE NO.: 104:22097a,22100a

TITLE: Copper complexes with quadridentate bis(pyrazolyl)thioether amine and tris(pyrazolyl)amine ligands. Structural characterization of the complexes isothiocyanato[tris(2-pyrazolylethyl)amine-NN2N2'N2'']copper(II) diisothiocyanatocuprate(I) and {bis[2-(3',5'-dimethylpyrazolyl)ethyl](2-methylthioethyl)amine-NN2N2'S}chlorocopper(II) chloride dihydrate

AUTHOR(S): Di Vaira, Massimo; Mani, Fabrizio

CORPORATE SOURCE: Dep. Chem., Univ. Florence, Florence, Italy

SOURCE: Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1972-1999) (1985), (11), 2327-32
CODEN: JCDTBI; ISSN: 0300-9246

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 19 Apr 1986

AB Reactions of simple Cu salts with the tripod quadridentate ligands L [L = tris(2-pyrazolylethyl)amine (L1), bis[2-(3',5'-dimethylpyrazolyl)ethyl][2-(methylthio)ethyl]amine (L2)] gave the complexes [CuXL1][BPh4] (X = Cl, Br, NCS), [CuClL1]2[CuCl4], [Cu(NCS)L][Cu(NCS)2] (I), [Cu(NCS)L2][BPh4].Me2CO, [CuClL2]Cl.2H2O (II), and [CuBrL2]3[CuBr3]Br.H2O. The crystal and mol. structures of I (L = L1) and II were determined by x-ray diffraction using the heavy-atom method and refined by full-matrix least squares to R 0.040 and 0.044 for 2518 and 1559 observed reflections, resp. I (L = L1) consists of isolated cations with the Cu in an approx. trigonal-bipyramidal environment of 5 N atoms and of layers formed by the [Cu(NCS)2]- anion, with pseudotetrahedral Cu(I) atoms. The Cu(II) atom in the cation of II is in a square-pyramidal environment of 1 S, 1 Cl, and 3 N atoms. L2 was prepared by the reaction of bis(2-chloroethyl)amine (which causes blistering) with K 3,5-

dimethylpyrazolate in THF, followed by reaction of the intermediate amine with Cl(CH2)2SMe in EtOH.

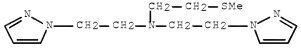
CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 28, 75

IT 101049-76-7P 101049-79-0P 101049-81-4P 101065-14-9P 101065-15-0P
101065-18-3P 101125-00-2P 101131-44-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 101131-44-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 101131-44-6 HCAPLUS

CN 1H-Pyrazole-1-ethanamine, N-[2-(methylthio)ethyl]-N-[2-(1H-pyrazol-1-yl)ethyl]- (CA INDEX NAME)



L47 ANSWER 21 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER:	1984:530693 HCAPLUS Full-text
DOCUMENT NUMBER:	101:130693
ORIGINAL REFERENCE NO.:	101:19885a,19888a
TITLE:	(Azolylmethyl)amines and their use in microbicidal agents
INVENTOR(S):	Oeckl, Siegfried; Schmitt, Hans Georg; Paulus, Wilfried; Genth, Hermann
PATENT ASSIGNEE(S):	Bayer A.-G. , Fed. Rep. Ger.
SOURCE:	Ger. Offen., 38 pp. CODEN: GWXXBX
DOCUMENT TYPE:	Patent
LANGUAGE:	German
FAMILY ACC. NUM. COUNT:	1

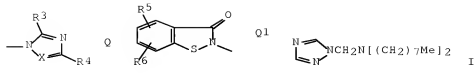
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3238006	A1	19840419	DE 1982-3238006	19821013 <--
US 4599427	A	19860708	US 1983-536929	19830928 <--
EP 106243	A1	19840425	EP 1983-109794	19830930 <--
EP 106243	B1	19860528		
R: BE, DE, FR, GB, IT, SE				
JP 59093058	A	19840529	JP 1983-188558	19831011 <--
JP 06029268	B	19940420		
CA 1243315	A1	19881018	CA 1983-438858	19831011 <--
PRIORITY APPLN. INFO.:			DE 1982-3238006 A	19821013 <--

OTHER SOURCE(S): CASREACT 101:130693

ED Entered STN: 13 Oct 1984

GI



AB R1R2NCH2R (R = Q, Q1; X = N, CR7; R1 = C1-24 aliphatic group, C3-12 cycloalkyl, C7-24 aralkyl, C1-24 aminoalkyl, C2-24 alkylenaminoalkyl, C6-18 aryl, C7-24 alkylaryl, C6-18 haloaryl, C1-24 alkoxy, C7-24 arylalkoxy, CH2R; R2 = H, R1; NR1R2 = 5- or 6-membered heterocyclyl; R3-R7 = H, halo, NO2, C1-24 alkyl, C3-12 cycloalkyl, C1-24 alkoxy, cyano, C7-24 aralkyl), useful as bactericides, fungicides, algicides, and slimicides, were prepared Thus, treating [Me(CH2)7]2NH and 1,2,4-triazole in CH2Cl2 or (ClCH2)2 with 30% HCHO at 30-35° gave 98% (triazolylmethyl)amine I. The min. inhibitory concentration of I for Alternaria tenuis was 50 μg/L, for Escherichia coli was 95 μg/L, for slime organisms 75 μg/L, and for a mixed culture of green, blue, and brown algae and diatoms the lethal concentration was 20 μg/L.

IC C07D249-08; C07D275-04; C07D401-06; C07D403-06; C07D413-06; A01N043-50; A01N043-64; A01N043-80; A01N043-00; C02F001-50; C09D005-14; C09J003-00

CC 28-10 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 5, 10

IT 23230-39-9P 23230-41-3P 23230-42-4P 23230-43-5P 23230-44-6P
76686-85-6P 76686-86-7P 91272-74-1P 91272-75-2P 91272-76-3P
91272-77-4P 91272-78-5P 91272-79-6P 91272-80-9P 91272-81-0P
91272-82-1P 91272-83-2P 91272-84-3P 91272-85-4P 91272-86-5P
91272-87-6P 91272-88-7P 91272-89-8P 91272-90-1P 91272-91-2P
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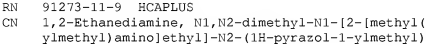
91273-08-4P 91273-09-5P 91273-10-8P 91273-11-9P
91273-12-0P 91273-13-1P 91273-14-2P 91273-15-3P 91273-16-4P
91273-17-5P 91273-18-6P 91273-19-7P 91273-20-0P 91273-22-2P
91273-23-3P 91273-24-4P 91273-26-6P 91273-30-2P 91273-31-3P
91273-32-4P 91273-33-5P 91273-34-6P 91273-35-7P 91273-36-8P
91273-37-9P 91273-39-1P 91274-94-1P 93597-03-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as biocide)

IT 91273-11-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as biocide)

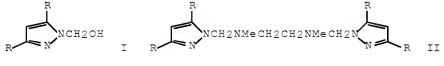
RN 91273-11-9 HCAPLUS

CN 1,2-Ethanediamine, N1,N2-dimethyl-N1-[2-[methyl(1H-pyrazol-1-ylmethyl)amino]ethyl]-N2-(1H-pyrazol-1-ylmethyl)- (CA INDEX NAME)

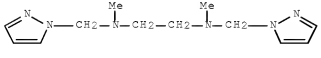


L47 ANSWER 22 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1983:160629 HCAPLUS Full-text
DOCUMENT NUMBER: 98:160629

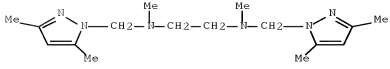
ORIGINAL REFERENCE NO.: 98:24379a,24382a
TITLE: Synthesis of some new pyrazole-containing chelating agents
AUTHOR(S): Driessen, Willem L.
CORPORATE SOURCE: Dep. Chem., State Univ. Leiden, Leiden, 2300 RA, Neth.
SOURCE: Recueil: Journal of the Royal Netherlands Chemical Society (1982), 101(12), 441-3
CODEN: RJRSDK; ISSN: 0165-0513
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 98:160629
ED Entered STN: 12 May 1984
GI



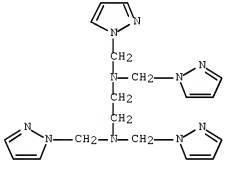
AB The (hydroxymethyl)pyrrazoles I (R = H, Me) underwent condensation with EtNH2, PhNH2, MeNHCH2CH2NHMe, H2NCH2CH2NH2, H2NCH2CH2NHCH2CH2NH2, (H2NCH2CH2NHCH2)2, and NH3 to give products in which all amine hydrogens were substituted by 1-pyrazolylmethyl groups, e.g. II.
CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
ST chelating agent pyrazolylmethylamine deriv; pyrazolylmethylamine deriv
IT 85264-34-2P 85264-35-3P 85264-36-4P 85264-37-5P 85264-38-6P 85264-39-7P 85264-40-0P 85264-41-1P 85264-42-2P 85264-43-3P 85264-44-4P 85264-45-5P 85264-46-6P 85264-47-7P 85264-48-8P 85264-49-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 85264-38-6P 85264-39-7P 85264-42-2P 85264-43-3P 85264-44-4P 85264-45-5P 85264-46-6P 85264-47-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 85264-38-6 HCAPLUS
CN 1,2-Ethanediamine, N1,N2-dimethyl-N1,N2-bis(1H-pyrazol-1-ylmethyl)- (CA INDEX NAME)



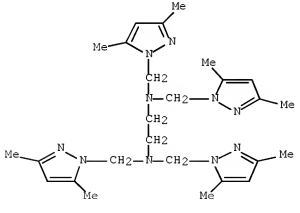
RN 85264-39-7 HCAPLUS
CN 1,2-Ethanediamine, N1,N2-bis[(3,5-dimethyl-1H-pyrazol-1-yl)methyl]-N1,N2-dimethyl- (CA INDEX NAME)



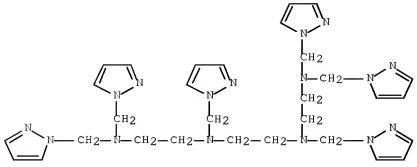
RN 85264-42-2 HCAPLUS
CN 1,2-Ethanediamine, N1,N1,N2,N2-tetrakis(1H-pyrazol-1-ylmethyl)- (CA INDEX NAME)



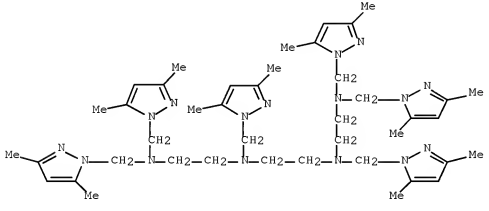
RN 85264-43-3 HCAPLUS
CN 1,2-Ethanediamine, N1,N1,N2,N2-tetrakis[(3,5-dimethyl-1H-pyrazol-1-yl)methyl]- (CA INDEX NAME)



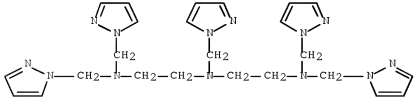
RN 85264-44-4 HCAPLUS
CN 1,2-Ethanediamine, N1,N2-bis[2-[bis(1H-pyrazol-1-ylmethyl)amino]ethyl]-N1,N2-bis(1H-pyrazol-1-ylmethyl)- (CA INDEX NAME)



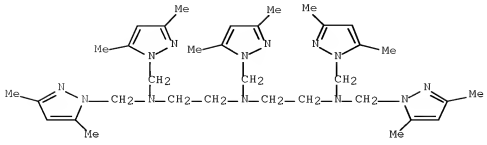
RN 85264-45-5 HCAPLUS
CN 1,2-Ethanediamine, N1,N2-bis[2-[bis[(3,5-dimethyl-1H-pyrazol-1-yl)methyl]amino]ethyl]-N1,N2-bis[(3,5-dimethyl-1H-pyrazol-1-yl)methyl]- (CA INDEX NAME)



RN 85264-46-6 HCAPLUS
CN 1,2-Ethanediamine, N1-[2-[bis(1H-pyrazol-1-ylmethyl)amino]ethyl]-N1,N2,N2-tris(1H-pyrazol-1-ylmethyl)- (CA INDEX NAME)



RN 85264-47-7 HCAPLUS
CN 1,2-Ethanediamine, N1-[2-[bis[(3,5-dimethyl-1H-pyrazol-1-yl)methyl]amino]ethyl]-N1,N2,N2-tris[(3,5-dimethyl-1H-pyrazol-1-yl)methyl]- (CA INDEX NAME)



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L47  ANSWER 23 OF 23  WPIX COPYRIGHT 2009        THOMSON REUTERS on STN
ACCESSION NUMBER:     2004-068858 [07]    WPIX
CROSS REFERENCE:      1996-221899; 1998-130312; 1998-240752; 1998-240943;
                      1998-240950; 1998-241072; 1998-397917; 1998-583442;
                      1999-080876; 1999-132432; 1999-142839; 1999-142962;
                      1999-302357; 1999-611065; 2000-052183; 2000-105073;
                      2000-136305; 2000-338767; 2000-505663; 2000-638498;
                      2001-272561; 2001-272673; 2001-391546; 2001-656196;
                      2002-061387; 2002-138760; 2002-156532; 2002-314807;
                      2002-463278; 2002-470122; 2002-625845; 2003-038162;
                      2003-329825; 2003-354490; 2003-656115; 2003-669409;
                      2003-742808; 2003-754498; 2003-765734; 2003-777476;
                      2003-811094; 2004-212114; 2004-223799; 2004-224691;
                      2004-236784; 2006-008320; 2008-C33816
DOC. NO. CPI:         C2004-028387 [07]
DOC. NO. NON-CPI:     N2004-055373 [07]
TITLE:                Production of metal-ligand compounds used in olefin
                      oligomerization, by synthesizing first and second metal
                      binding ligands in respective regions on substrate and
                      delivering respective metal ion to each metal binding
                      ligand
DERWENT CLASS:        A60; B04; E19; J04; S03
INVENTOR:             BOUSSIE T; GOLDWASSER I; MCFARLAND E; MURPHY V; POWERS T;
                      TURNER H; VAN BEEK J A M; WEINBERG W H
PATENT ASSIGNEE:      (SYMY-N) SYMYX TECHNOLOGIES INC
COUNTRY COUNT:        1

PATENT INFORMATION:

      PATENT NO      KIND DATE     WEEK     LA  PG          MAIN IPC
      ------------------------------------------------------------------
      US 20030100119 A1 20030529 (200407)* EN  64[30]                    <--

APPLICATION DETAILS:

      PATENT NO      KIND                APPLICATION    DATE
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US 20030100119 A1	Div Ex	US 1994-327513 19941018
US 20030100119 A1	Provisional	US 1996-16102P 19960723
US 20030100119 A1	Provisional	US 1996-28106P 19961009
US 20030100119 A1	Provisional	US 1996-29255P 19961025
US 20030100119 A1	Provisional	US 1997-35366P 19970110
US 20030100119 A1	Provisional	US 1997-48987P 19970609
US 20030100119 A1	CIP of	US 1998-127660 19980731
US 20030100119 A1	Cont of	US 1999-337047 19990621
US 20030100119 A1		US 2002-269362 20021011

FILING DETAILS:

PATENT NO	KIND	PATENT NO
US 20030100119 A1	Div ex	US 5985356 A
US 20030100119 A1	CIP of	US 6420179 B

PRIORITY APPLN. INFO: US 2002-269362 20021011
US 1994-327513 19941018
US 1996-16102P 19960723
US 1996-28106P 19961009
US 1996-29255P 19961025
US 1997-35366P 19970110
US 1997-48987P 19970609
US 1998-127660 19980731
US 1999-337047 19990621

INT. PATENT CLASSIF.:
IPC RECLASSIF.: G01N0001-10 [I,A]; G01N0001-10 [I,C]
USCLASS NCLM: 436/037.000
NCLS: 436/073.000; 436/180.000

BASIC ABSTRACT:

US 20030100119 A1 UPAB: 20060203

NOVELTY - Production of an array of metal ligand compounds (A) comprises synthesizing first and second metal binding ligands in respective regions on a substrate and delivering respective metal ions to each metal binding ligand to form first and second metal ligand compounds.

DETAILED DESCRIPTION - INDEPENDENT CLAIMS are also included for:

(a) preparing a polymer blend by contacting at least two (A) with a cocatalyst and a monomer, and

(b) polymerizing olefins, diolefins, and acetylenically unsaturated monomers by contacting (A) with a cocatalyst and a monomer.

USE - Used for preparing an array of (A) useful for an organic transformation reaction requiring Lewis acidic sites, e.g. stereo-selective coupling reactions, olefin oligomerization reactions or olefin polymerization reactions. (A) Are used to prepare polymer blend or to polymerize olefins, diolefins or acetylenically unsaturated monomers.

ADVANTAGE - The method accelerates the rate discovering and optimizing catalytic process, and rapidly characterizes each member to identify compounds with specific, desired properties, e.g. polymerization characteristics, mechanical, optical, physical or morphological property, lifetime, stability, selectivity, conversion efficiency, or activity of (A).

MANUAL CODE: CPI: A02-A06D; A04-G01A; B05-A03B; B07-D08; B10-A20; B11-C01A; B11-C01B; E05-L02C; E05-M; E11-K01; E11-K02; J04-E04
EPI: S03-E13D

TECH

INORGANIC CHEMISTRY - Preferred Method: The method also involves activating both metal-ligands with respective activator to form first and second activated (A). The synthesizing step also involves sequentially

synthesizing first and second components of each metal binding ligand. The method also involves screening the array of (A) for useful properties using scanned mass spectrometry, chromatography, ultraviolet imaging, visible imaging, infrared imaging, electromagnetic imaging, ultraviolet spectroscopy, visible spectroscopy, infrared spectroscopy, electromagnetic spectroscopy, or acoustical methods.

The array of (A) is further modified by reaction with an ion-exchange activator to produce an array of ligand-stabilized cationic aluminum reagents.

Preferred Components: The activated (A) are organometallic compounds, homogeneous catalysts or heterogeneous catalysts. The first and second metal-ligand compounds are activated-free catalysts, which are homogeneous or heterogeneous catalysts. The metal-binding ligands are neutral bidentate ligands, mono-anionic bidentate ligands, chelating diamine ligands comprising 1,2-diamine ligands, salen ligands or ancillary ligands. The first and second metal ions are each transition metals comprising palladium, nickel, platinum, iridium, rhodium, chromium, molybdenum, tungsten, or cobalt. The first and second activators include methylaluminaoxane (MAO), (Q)+(NCA)- (NCA = non-coordinating anions), (H(OEt2)+(BAr4)- or (H(OEt2))+(B(C6F5)4)-.

The metal-binding ligands are (2,2) or (2,1) ligands that are respectively contacted with a main group of metal alkyl complex such that they are in the mono- or di-protic form. The ligand-stabilized cationic aluminum reagents can be used as catalyst for the transformation reaction.

The metal-binding ligands have a coordination number (CN) comprising 1-3 or a charge comprising 0, -1 to -4. They have a CN with corresponding charge consisting of CN = 2, charge = -2, -1, -3 or neutral; CN = 1, charge = -1,-2 or -3; or CN = 3, charge = -1 or -3.

When metal-binding ligands are ancillary ligands, each has a charge that is greater than the coordination number, neutral bidentate ligands, each of the transition metal ions is stabilized by a labile neutral Lewis base,) chelating diamine ligands each of the transition metal ions is a Group 10 transition metal, or monoanionic bidentate ligands, each of the transition metal ions is stabilized by a labile anionic leaving group ligand. The activators form counter-ions after activation.

The metal-binding ligands are directly attached to the substrate or to the first and second synthesis support on the substrate, or attached to the substrate through first and second linker groups. The substrate is a porous or non-porous substrate. The array can be screened simultaneously, serially, or in a spatially selective manner.

Each (A) is synthesized in an area of less than 25 cm2, preferably less than 1 mm2, especially less than 1micro-m2. At least 10 (especially at least 10 power 6) different (A) are synthesized on the substrate.

ORGANIC CHEMISTRY - Preferred Components: The metal alkyl complex is trialkylaluminum complex. The ion-exchange activator is (PhNMe2H)(B(C6F5)4).

ABEX EXAMPLE - (2,4,6-Me)2N,N-dimethyl-4-aminoazobenzene(Me)EtPh (0.50 g) and (ethylene glycol dimethyl ether)NiBr2 (0.36 g) were dissolved in dry CH2Cl2 (8 ml) under nitrogen and stirred at room temperature for 8 hours. The obtained solution was concentrated and the residue recrystallized from CH2Cl2/hexane to give (2,4,6-Me)2N,N-dimethyl-4-aminoazobenzene(Me)EtPh nickel (II) dibromide (53%).

AN.S DCR-776360

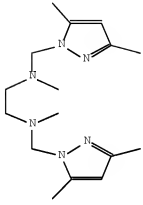
SDCN RABNX7

CM 1

CM 2

Ni

CM 3



AN.S DCR-776360
SDCN RABNX7

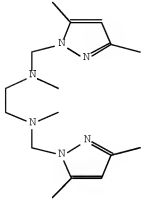
CM 1

Br

CM 2

Ni

CM 3



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LAST RELOADED: Jun 19, 2009 (20090619/UP).

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L48  ANSWER 1 OF 5  HCAPLUS  COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER:        2008:732443  HCAPLUS  Full-text
DOCUMENT NUMBER:         149:257825
TITLE:                   Synthesis of new palladium(II) complexes containing
                         tetradentate-nitrogen donor ligands: Combined
                         structural studies by NMR spectroscopy and X-ray
                         crystallography
AUTHOR(S):               Espinal, Monica; Pons, Josefina; Garcia-Anton, Jordi;
                         Solans, Xavier; Font-Bardia, Merce; Ros, Josep
CORPORATE SOURCE:        Departament de Quimica, Unitat de Quimica Inorganica,
                         Universitat Autonoma de Barcelona, Bellaterra,
                         Barcelona, 08193, Spain
SOURCE:                  Inorganica Chimica Acta (2008), 361(9-10), 2648-2658
                         CODEN: ICHAA3; ISSN: 0020-1693
PUBLISHER:               Elsevier B.V.
DOCUMENT TYPE:           Journal
LANGUAGE:                English
OTHER SOURCE(S):         CASREACT 149:257825
ED   Entered STN:  19 Jun 2008
AB   Treatment of the tetradentate (NN'N'N) N-alkylaminopyrazole ligands 3,6-
     dimethyl-1,8-(3,5-dimethyl-1-pyrazolyl)-3,6-diazaoctane (ddad) and 1,4-bis[2-
     (3,5-dimethyl-1-pyrazolyl)ethyl]piperazine (bedp) with [PdCl2(MeCN)2] in a 1:1
     M/L ratio in MeCN produces [Pd2Cl4(L)] and [PdCl2(L)] (L = ddad and bedp).
     Treatment of the corresponding complex [PdCl2(L)] (L = ddad, bedp) in the
     presence of AgBF4 in CH2Cl2/MeOH (2:1) or NaBF4 in MeCN gives [Pd(L)](BF4)2.
     The Pd(II) complexes were characterized by elemental analyses, conductivity
     measurements, IR and 1H and 13C{1H} NMR spectroscopies when possible.  The x-
     ray structure of [Pd(ddad)]Cl2·3H2O was determined  The Pd(II) is coordinated
```

to the ddad ligand by two N atoms of pyrazolyl groups and two N atoms of the amine groups, in a slightly distorted square-planar geometry.

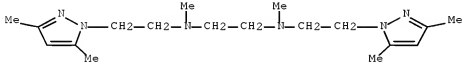
CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 75

IT 139775-87-4 139775-88-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(complexation with palladium)

IT 139775-87-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(complexation with palladium)

RN 139775-87-4 HCAPLUS

CN 1,2-Ethanediamine, N1,N2-bis[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]-N1,N2-dimethyl- (CA INDEX NAME)



REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L48 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2008:261803 HCAPLUS Full-text

DOCUMENT NUMBER: 150:144351

TITLE: Synthesis of 1-(2-aminoethyl)pyrazoles under phase-transfer catalysis

AUTHOR(S): Attaryan, O. S.; Baltayan, A. O.; Sagatelyan, R. E.; Takmazyan, K. Ts.

CORPORATE SOURCE: Institute of Organic Chemistry, National Academy of Sciences of Armenia, Yerevan, 375091, Armenia

SOURCE: Russian Journal of General Chemistry (2008), 78(1), 136-138
CODEN: RJGCEK; ISSN: 1070-3632

PUBLISHER: Pleiades Publishing, Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 03 Mar 2008

AB Alkylation of pyrazoles with 2-chloroethylamine was performed under conditions of phase-transfer catalysis. Depending on the substrate acidity, the electrophilic substitution process may be accompanied by dehydrochlorination of the alkylating agent, so that 6 equiv of 2-chloroethylamine should be used in the alkylation of 3,5-dimethylpyrazole.

CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))

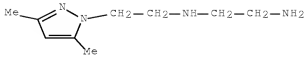
IT 62821-88-9P 62821-90-3P 101395-71-5P, 1H-Pyrazole-1-ethanamine
101395-72-6P 511513-23-8P 1101099-34-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of pyrazoleethanamine by alkylation of pyrazole with chloroethanamine under phase-transfer catalysis)

IT 511513-23-8P 1101099-34-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of pyrazoleethanamine by alkylation of pyrazole with chloroethanamine under phase-transfer catalysis)

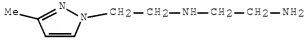
RN 511513-23-8 HCAPLUS

CN 1,2-Ethanediamine, N1-[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]- (CA INDEX

NAME)

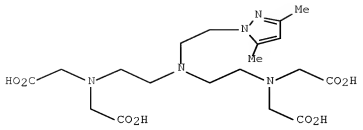


RN 1101099-34-6 HCAPLUS
CN 1,2-Ethanediamine, N1-[2-(3-methyl-1H-pyrazol-1-yl)ethyl]- (CA INDEX NAME)



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L48 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2006:612137 HCAPLUS Full-text
DOCUMENT NUMBER: 146:286880
TITLE: Experimental and theoretical study of lanthanide complexes based on linear and macrocyclic polyaminopolycarboxylic acids with pyrazolylethyl arms
AUTHOR(S): Perez-Mayoral, Elena; Soriano, Elena; Cerdan, Sebastian; Ballesteros, Paloma
CORPORATE SOURCE: Laboratorio de Sintesis Organica e Imagen Molecular por Resonancia Magnetica, Instituto Universitario de Investigacion, Facultad de Ciencias, UNED, Madrid, E-28040, Spain
SOURCE: Proceedings of ECSOC-9, International Electronic Conference on Synthetic Organic Chemistry, 9th, Nov. 1-30, 2005 (2005), C003/1-C003/11. Editor(s): Seijas, Julio A.; Vazquez Tato, M. Pilar. Molecular Diversity Preservation International: Basel, Switz. CODEN: 69IFGU; ISBN: 3-906980-16-2
DOCUMENT TYPE: Conference; (computer optical disk)
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:286880
ED Entered STN: 26 Jun 2006
GI



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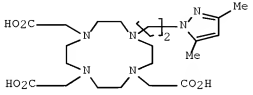


II

AB The preparation and magnetic relaxometric properties of gadolinium complexes with polyaminopolycarboxylic acids with pyrazolylethyl arms (I, II) is described. Optimized geometries for the Gd(L)(H2O) complexes (L = I, II, diethylenetriamine pentaacetic acid (TPA), and 1,4,7,10-tetraazacyclododecane-1,4,7,10-tetraacetic acid) (DOTA) were calculated from DFT methods.

CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 28, 65, 77

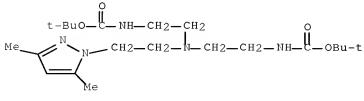
IT 96-32-2 67000-35-5 117499-16-8 149353-23-1 885689-63-4
927431-26-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of polyaminopolycarboxylic acid with pyrazolylethyl arms)

IT 885678-69-3P 885689-50-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and complexation with gadolinium(III))

IT 885689-63-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of polyaminopolycarboxylic acid with pyrazolylethyl arms)

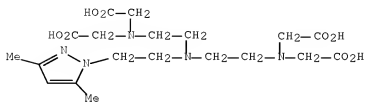
RN 885689-63-4 HCAPLUS

CN 10-Oxa-2,5,8-triazadodecanoic acid, 5-[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]-11,11-dimethyl-9-oxo-, 1,1-dimethylethyl ester (CA INDEX NAME)



IT 885689-50-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(preparation and complexation with gadolinium(III))
RN 885689-50-9 HCAPLUS
CN Glycine, N,N'-[[[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]imino]di-2,1-ethanediyl]bis[N-(carboxymethyl)-, sodium salt (1:4) (CA INDEX NAME)



●4 Na

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L48 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2006:601860 HCAPLUS Full-text
DOCUMENT NUMBER: 146:219353
TITLE: Experimental and theoretical study of lanthanide complexes based on linear and macrocyclic polyaminopolycarboxylic acids containing pyrazolylethyl arms
AUTHOR(S): Perez-Mayoral, Elena; Soriano, Elena; Cerdan, Sebastian; Ballesteros, Paloma
CORPORATE SOURCE: Laboratorio de Sintesis Organica e Imagen Molecular por Resonancia Magnetica, Instituto Universitario de Investigacion, Facultad de Ciencias, UNED, Madrid, E-28040, Spain
SOURCE: Molecules (2006), 11(5), 345-356
CODEN: MOLEFW; ISSN: 1420-3049
URL: http://mdpi.org/subscribers/molecules/papers/1105-0345.pdf
PUBLISHER: Molecular Diversity Preservation International
DOCUMENT TYPE: Journal; (online computer file)
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:219353
ED Entered STN: 22 Jun 2006
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB We report the synthesis of two novel Gd(III)-complexes Gd(L) and Gd(L') derived from linear and macrocyclic polyaminopolycarboxylic acids (I) = H4L and (II) = H3L', resp., and a study of their relaxivity properties. Optimized geometries of the gadolinium complexes also are reported. The relationships between the exptl. and theor. results have provided interesting information about the kinetic and thermodn. stability of these complexes.
CC 78-7 (Inorganic Chemicals and Reactions)

Section cross-reference(s): 28, 65, 67, 77

IT 885689-63-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reactant for preparation of N,N'-[[[(dimethyl-pyrazolyl)ethyl]imino]diethanediyl]bis[N-(carboxymethyl)]glycine)

IT 885689-50-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reactant for preparation of gadolinium N,N'-[[[(dimethyl-pyrazolyl)ethyl]imino]diethanediyl]bis[N-(carboxymethyl)]glycine complex)

IT 885689-67-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(reactant for preparation of N,N'-[[[(dimethyl-pyrazolyl)ethyl]imino]diethanediyl]bis[N-(carboxymethyl)]glycine)

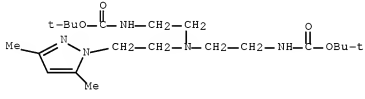
IT 885689-63-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reactant for preparation of N,N'-[[[(dimethyl-pyrazolyl)ethyl]imino]diethanediyl]bis[N-(carboxymethyl)]glycine)

RN 885689-63-4 HCAPLUS

CN 10-Oxa-2,5,8-triazadodecanoic acid, 5-[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]-11,11-dimethyl-9-oxo-, 1,1-dimethylethyl ester (CA INDEX NAME)



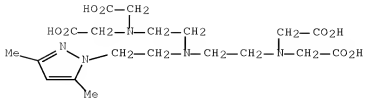
IT 885689-50-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

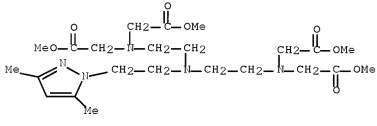
(preparation and reactant for preparation of gadolinium N,N'-[[[(dimethyl-pyrazolyl)ethyl]imino]diethanediyl]bis[N-(carboxymethyl)]glycine complex)

RN 885689-50-9 HCAPLUS

CN Glycine, N,N'-[[[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]imino]di-2,1-ethanediyl]bis[N-(carboxymethyl)-, sodium salt (1:4) (CA INDEX NAME)



IT 885689-67-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(reactant for preparation of N,N'-[[[(dimethyl-pyrazolyl)ethyl]imino]diethanediyl]bis[N-(carboxymethyl)]glycine)
RN 885689-67-8 HCAPLUS
CN 2-Oxa-5,8,11-triazatridecan-13-oic acid, 8-[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]-5,11-bis(2-methoxy-2-oxoethyl)-3-oxo-, methyl ester (9CI) (CA INDEX NAME)



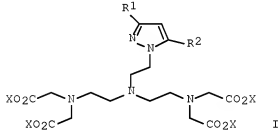
REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L48 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2006:469891 HCAPLUS Full-text
DOCUMENT NUMBER: 144:459915
TITLE: Preparation of (pyrazolylethyl)diethylenetriaminetetraacetate heterocyclic ligands and their gadolinium(III) complexes with biomedical applications
INVENTOR(S): Ballesteros Garcia, Paloma
PATENT ASSIGNEE(S): Universidad Nacional De Educacion A Distancia (U.N.E.D.), Spain
SOURCE: PCT Int. Appl., 23 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Spanish
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006051143	A1	20060518	WO 2005-ES602	20051107

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

ES 2253114 A1 20060516 ES 2004-2679 20041108
ES 2253114 B1 20070701
PRIORITY APPLN. INFO.: ES 2004-2679 A 20041108
OTHER SOURCE(S): MARPAT 144:459915
ED Entered STN: 19 May 2006
GI



AB The invention relates to compds. DTPA-like ligands (I) and their paramagnetic complexes of Gd(III) and other lanthanides which may be used as contrast agents for magnetic resonance imaging. More specifically, the invention relates to compds. I, wherein R1 and/or R2 are hydrogens, Me groups, nitro groups and amino groups. The invention further relates to a method of obtaining said compds. from the corresponding bromoethylpyrazoles, comprising the following steps: 1) alkylation of the original amine; 2) deprotection of the tert-butoxycarbonylamino groups; 3) alkylation of the amino groups with Me bromoacetate; and, finally, 4) basic hydrolysis which produces the tetrasodium salt. The invention relates to complexes of Gd(III) and of other lanthanides derived from compds. I, to the method of obtaining said complexes and to the exptl. and clin. use of same in the production of contrast agents for clin. diagnosis by magnetic resonance imaging. Thus, ligands I (Na4L; X = Na; R1, R2 = H, H; Me, Me; NO2, H; NH2, H) were prepared and complexed with gadolinium to give Na[GdL] complexes. The relaxivities of these gadolinium were measured to determine their suitability as MRI contrast agents.

CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 8, 28

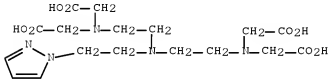
IT 885689-48-5P 885689-50-9P 885689-52-1P 885689-54-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(ligand; preparation of (pyrazolylethyl)diethylenetriaminetetraacetate heterocyclic ligands and their gadolinium(III) complexes for use as MRI

contrast agents)

IT 885689-57-6P 885689-59-8P 885689-63-4P
885689-65-6P 885689-67-8P 885689-69-0P 885689-71-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (pyrazolylethyl)diethylenetriaminetetraacetate heterocyclic ligands and their gadolinium(III) complexes for use as MRI contrast agents)

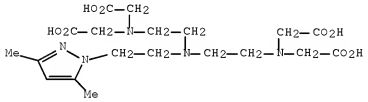
IT 885689-48-5P 885689-50-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(ligand; preparation of (pyrazolylethyl)diethylenetriaminetetraacetate heterocyclic ligands and their gadolinium(III) complexes for use as MRI contrast agents)

RN 885689-48-5 HCAPLUS
CN Glycine, N,N'-[[[2-(1H-pyrazol-1-yl)ethyl]imino]di-2,1-ethanediyl]bis[N-(carboxymethyl)-, tetrasodium salt (9CI) (CA INDEX NAME)



●4 Na

RN 885689-50-9 HCAPLUS
CN Glycine, N,N'-[[[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]imino]di-2,1-ethanediyl]bis[N-(carboxymethyl)-, sodium salt (1:4) (CA INDEX NAME)

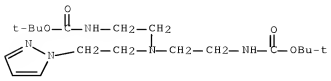


●4 Na

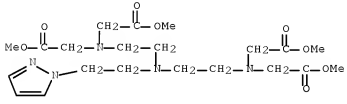
IT 885689-57-6P 885689-59-8P 885689-63-4P
885689-67-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (pyrazolylethyl)diethylenetriaminetetraacetate heterocyclic ligands and their gadolinium(III) complexes for use as MRI contrast agents)

RN 885689-57-6 HCAPLUS
CN 10-Oxa-2,5,8-triazadodecanoic acid, 11,11-dimethyl-9-oxo-5-[2-(1H-pyrazol-1-yl)ethyl]-, 1,1-dimethylethyl

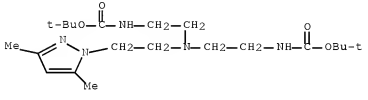
ester (CA INDEX NAME)



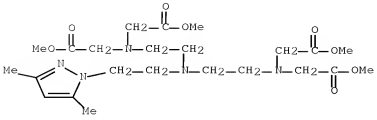
RN 885689-59-8 HCAPLUS
CN 2-Oxa-5,8,11-triazatridecan-13-oic acid, 5,11-bis(2-methoxy-2-oxoethyl)-3-oxo-8-[2-(1H-pyrazol-1-yl)ethyl]-, methyl ester (9CI) (CA INDEX NAME)



RN 885689-63-4 HCAPLUS
CN 10-Oxa-2,5,8-triazadodecanoic acid, 5-[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]-11,11-dimethyl-9-oxo-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 885689-67-8 HCAPLUS
CN 2-Oxa-5,8,11-triazatridecan-13-oic acid, 8-[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]-5,11-bis(2-methoxy-2-oxoethyl)-3-oxo-, methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L10               STR
L12            90 SEA FILE=REGISTRY SUB=L7 SSS FUL L10
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L15               QUE  SPE=ON  ABB=ON  PLU=ON  REGO, I?/AU,AUTH
L16               QUE  SPE=ON  ABB=ON  PLU=ON  CORREIA, J?/AU,AUTH
L17               QUE  SPE=ON  ABB=ON  PLU=ON  PAULO, A?/AU,AUTH
L18               QUE  SPE=ON  ABB=ON  PLU=ON  ALVES, S?/AU,AUTH
L19               QUE  SPE=ON  ABB=ON  PLU=ON  VITOR, R?/AU,AUTH
L20               QUE  SPE=ON  ABB=ON  PLU=ON  MALLINCKRODT/CS,SO,PA
L22               QUE  SPE=ON  ABB=ON  PLU=ON  BIOMOLECUL? OR (BIO(1W)MOLEC
                  UL?) OR (BIOLOGIC?(3A)MOLECUL?)
L23               QUE  SPE=ON  ABB=ON  PLU=ON  CHELAT?
L24               QUE  SPE=ON  ABB=ON  PLU=ON  "CHELATING AGENTS"+PFT,OLD,N
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L25            46 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L12
L26            19 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L25 AND (L22 OR L23
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L27            46 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  (L25 OR L26)
L28            18 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L27 AND (L14 OR L15
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L16               QUE  SPE=ON  ABB=ON  PLU=ON  CORREIA, J?/AU,AUTH
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L19               QUE  SPE=ON  ABB=ON  PLU=ON  VITOR, R?/AU,AUTH
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L22               QUE  SPE=ON  ABB=ON  PLU=ON  BIOMOLECUL? OR (BIO(1W)MOLEC
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L23               QUE  SPE=ON  ABB=ON  PLU=ON  CHELAT?
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                  L33/DCR
L35             2 SEA FILE=WPIX SPE=ON  ABB=ON  PLU=ON  L34 AND (L22 OR L23)
L36             3 SEA FILE=WPIX SPE=ON  ABB=ON  PLU=ON  (L34 OR L35)
L37             1 SEA FILE=WPIX SPE=ON  ABB=ON  PLU=ON  L36 AND (L14 OR L15 OR
                  L16 OR L17 OR L18 OR L19 OR L20)


=> d que nos 139
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L7            827 SEA FILE=REGISTRY SSS FUL L5
L10               STR
L12            90 SEA FILE=REGISTRY SUB=L7 SSS FUL L10
L39             0 SEA FILE=MEDLINE SPE=ON  ABB=ON  PLU=ON  L12


=> d que nos 141
L5                STR
L7            827 SEA FILE=REGISTRY SSS FUL L5
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L10             STR
L12          90 SEA FILE=REGISTRY SUB=L7 SSS FUL L10
L41           0 SEA FILE=EMBASE SPE=ON  ABB=ON  PLU=ON  L12


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     (FILE 'BIOSIS, CABA, AGRICOLA, BIOTECHNO, DRUGU, VETU' ENTERED AT
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=> d que nos l42
L5              STR
L7          827 SEA FILE=REGISTRY SSS FUL L5
L10             STR
L12          90 SEA FILE=REGISTRY SUB=L7 SSS FUL L10
L42           0 SEA L12


=> d his l44

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     BIOENG, BIOTECHNO, BIOTECHDS, DRUGU, DRUGB, VETU, VETB, SCISEARCH,
     CONFSCI, DISSABS, RDISCLOSURE' ENTERED AT 13:31:47 ON 25 JUN 2009)
L44          20 S L43 AND L14-L20

=> d que l44
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L15             QUE  SPE=ON  ABB=ON  PLU=ON  REGO, I?/AU,AUTH
L16             QUE  SPE=ON  ABB=ON  PLU=ON  CORREIA, J?/AU,AUTH
L17             QUE  SPE=ON  ABB=ON  PLU=ON  PAULO, A?/AU,AUTH
L18             QUE  SPE=ON  ABB=ON  PLU=ON  ALVES, S?/AU,AUTH
L19             QUE  SPE=ON  ABB=ON  PLU=ON  VITOR, R?/AU,AUTH
L20             QUE  SPE=ON  ABB=ON  PLU=ON  MALLINCKRODT/CS,SO,PA
L23             QUE  SPE=ON  ABB=ON  PLU=ON  CHELAT?
L43         769 SEA ?PYRAZOL?/IT,TI,CC,CT,ST,STP AND L23/IT,TI,CC,CT,ST,STP
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=> dup rem l28 l37 l39 l41 l42 l44
L39 HAS NO ANSWERS
L41 HAS NO ANSWERS
L42 HAS NO ANSWERS
DUPLICATE IS NOT AVAILABLE IN 'RDISCLOSURE'.
ANSWERS FROM THESE FILES WILL BE CONSIDERED UNIQUE
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PROCESSING COMPLETED FOR L39
PROCESSING COMPLETED FOR L41
PROCESSING COMPLETED FOR L42
PROCESSING COMPLETED FOR L44
L49          21 DUP REM L28 L37 L39 L41 L42 L44 (18 DUPLICATES REMOVED)
                ANSWERS '1-18' FROM FILE HCAPLUS
                ANSWER '19' FROM FILE EMBASE
                ANSWERS '20-21' FROM FILE SCISEARCH


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FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Jun 19, 2009 (20090619/UP).
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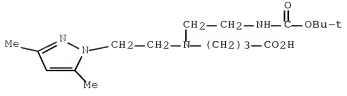
L49 ANSWER 1 OF 21 HCAPLUS COPYRIGHT 2009 ACS on STN DUPLICATE 1
ACCESSION NUMBER: 2008:1207034 HCAPLUS Full-text
DOCUMENT NUMBER: 150:20350
TITLE: Synthesis, characterization, and evaluation of a novel 99mTc(CO)3 pyrazolyl conjugate of a peptide nucleic acid sequence
AUTHOR(S): Xavier, Catarina; Giannini, Clelia; Gano, Lurdes; Maiorana, Stefano; Alberto, Roger; Santos, Isabel
CORPORATE SOURCE: Unidade de Ciencias Quimicas e Radiofarmaceuticas, Instituto Tecnologico e Nuclear, Sacavem, 2686-953, Port.
SOURCE: JBIC, Journal of Biological Inorganic Chemistry (2008), 13(8), 1335-1344
CODEN: JJBCFA; ISSN: 0949-8257
PUBLISHER: Springer GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 08 Oct 2008
AB The 16-mer peptide nucleic acid sequence H-A GAT CAT GCC CGG CAT-Lys-NH2 (1), which is complementary to the translation start region of the N-myc oncogene mRNA, was synthesized and conjugated to a pyrazolyl diamine bifunctional chelator (pz). The novel conjugate pz-A GAT CAT GCC CGG CAT-Lys-NH2 (2) was labeled with technetium tricarbonyl, yielding quant. the complex fac-[99mTc(CO)3(κ3-pz-A GAT CAT GCC CGG CAT-Lys-NH2)]2+ (4). Complex 4 was obtained with high radiochem. purity and high specific activity, revealing high stability in human serum and in cell culture medium. The identity of 4 was confirmed by comparing its reversed-phase high performance liquid chromatog. profile with that of the rhenium analog fac-[Re(CO)3(κ3-pz-A GAT CAT GCC CGG CAT-Lys-NH2)]2+ (3), prepared by conjugation of fac-[Re(CO)3(3,5-Me2pz(CH2)2N((CH2)3COOH)(CH2)2NH2)]+ to 1, using solid-phase techniques. UV melting expts. of 1 and 3 with the complementary DNA sequence led to the formation of stable duplexes, indicating that the conjugation of 1 to the pyrazolyl chelator and to the metal fragment fac-[M(CO)3]+ did not affect the recognition of the complementary sequence as well as the duplex stability. For a first screening, SH-SY5Y human neuroblastoma cells, which express N-myc, were treated with 4. The results show that 4 internalizes (7% of the activity goes into the cells, after 4 h at 37°), presenting also a relatively high cellular retention (only 40% of internalized activity is released from the cells after 5 h).
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 8, 78
IT Nucleic acid hybridization
(DNA-PNA; solid-phase preparation of peptide nucleic acid sequences, their conjugates with pyrazolyl chelator, and complexes with rhenium and 99-technetium)
IT Imaging agents
(solid-phase preparation of peptide nucleic acid sequences, their conjugates
with pyrazolyl chelator, and complexes with rhenium and 99-technetium)
IT Peptide nucleic acids
RL: BSU (Biological study, unclassified); PRP (Properties); RCT

(Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(solid-phase preparation of peptide nucleic acid sequences, their conjugates
with pyrazolyl chelator, and complexes with rhenium and 99-technetium)
IT 1089234-29-6P
RL: BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(solid-phase preparation of peptide nucleic acid sequences, their conjugates
with pyrazolyl chelator, and complexes with rhenium and 99-technetium)
IT 1089234-31-0 1089234-32-1
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(solid-phase preparation of peptide nucleic acid sequences, their conjugates
with pyrazolyl chelator, and complexes with rhenium and 99-technetium)
IT 1089234-26-3P 1089234-28-5P
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(solid-phase preparation of peptide nucleic acid sequences, their conjugates
with pyrazolyl chelator, and complexes with rhenium and 99-technetium)
IT 1089234-27-4P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(solid-phase preparation of peptide nucleic acid sequences, their conjugates
with pyrazolyl chelator, and complexes with rhenium and 99-technetium)
IT 163932-31-8 782501-78-4 945384-90-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(solid-phase preparation of peptide nucleic acid sequences, their conjugates
with pyrazolyl chelator, and complexes with rhenium and 99-technetium)
IT 1089234-30-9DP, resin-bound
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(solid-phase preparation of peptide nucleic acid sequences, their conjugates
with pyrazolyl chelator, and complexes with rhenium and 99-technetium)
IT 782501-78-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(solid-phase preparation of peptide nucleic acid sequences, their conjugates
with pyrazolyl chelator, and complexes with rhenium and 99-technetium)
RN 782501-78-4 HCAPLUS
CN Butanoic acid, 4-[[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl][2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]- (CA INDEX NAME)



REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

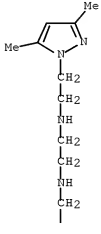
L49 ANSWER 2 OF 21 HCAPLUS COPYRIGHT 2009 ACS on STN DUPLICATE 2
ACCESSION NUMBER: 2008:521195 HCAPLUS Full-text
DOCUMENT NUMBER: 150:578080
TITLE: Pyrazolyl-diamine ligands that bear anthracenyl moieties and their rhenium(I) tricarbonyl complexes: synthesis, characterization and DNA-binding properties
AUTHOR(S): Vitor, Rute F.; Correia, Isabel; Videira, Margarida; Marques, Fernanda; Paulo, Antonio ; Pessoa, Joao Costa; Viola, Giampietro; Martins, Gabriel G.; Santos, Isabel
CORPORATE SOURCE: Departamento de Quimica, ITN, Sacavem, 2686-953, Port.
SOURCE: ChemBioChem (2008), 9(1), 131-142
CODEN: CBCHFX; ISSN: 1439-4227
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 30 Apr 2008
AB Two novel families of pyrazolyl-diamine ligands that bear an anthracen-9-yl group as a DNA-binding fragment, pz*(CH2)2NH(CH2)2NHCH2-9-anthryl (pz* = pz (L1), 3,5-Me2pz (L2)) and pz*(CH2)2NH(CH2)2NH2 (pz* = 4-(9-anthrylmethyl)pz (L3), 3,5-Me2-4-(9-anthrylmethyl)pz (L4)), were prepared and fully characterized. In the case of L2-L4, the evaluation of their coordination capability towards the fac-[Re(CO)3]+ core gave the organometallic complexes fac-[Re(CO)3{3,5-Me2pz(CH2)2NH(CH2)2NHCH2-9-anthryl}]Br (7) and fac-[Re(CO)3{4-(9-anthrylmethyl)pz*(CH2)2NH(CH2)2NH2}]Br (pz* = pz (8), 3,5-Me2pz (9)). The interaction of the novel pyrazole-diamine ligands and the rhenium(I) complexes with calf thymus (CT) DNA was studied with a variety of spectroscopic techniques (UV-visible, fluorescence, CD and linear dichroism (LD)). All of the evaluated compds. have a moderate affinity to CT DNA (3.46 + 103 < Kb < 1.95 + 104), but the binding mode depends on the position of the chromophore in the framework of the pyrazolyl-diamine ligands. LD measurements showed that L1 and L2 act as DNA intercalators, but complex 7 intercalates only partially. By contrast, the compds. with the anthracenyl group at the 4-position of the azolyl ring (L3, L4 and 9) do not intercalate, and behave more like DNA groove binders. Fluorescence microscopy studies demonstrated that complexes 7 and 9 can target the nucleus of murine B16-F1 melanoma cells, and appear to be promising platforms for the further design of radiopharmaceuticals for targeted radiotherapy.
CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 6, 28
IT 944389-67-7P 1152004-05-1P 1152004-07-3P
1152004-10-8P
RL: BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation, complexation with rhenium(I), and DNA binding)

IT 107-15-3, Ethylenediamine, reactions 109-84-2, 2-Hydroxyethylhydrazine 123-54-6, Acetylacetone, reactions 642-31-9, 9-Anthracenecarboxaldehyde 2417-77-8, 9-Bromomethylanthracene 58353-41-6, 2-(9-Anthrylmethyl)propane-1,3-diol 511513-23-8 782501-70-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant for preparation of substituted pyrazolyldiamine)

IT 1152004-05-1P 1152004-07-3P
RL: BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation, complexation with rhenium(I), and DNA binding)

RN 1152004-05-1 HCAPLUS
CN 1,2-Ethanediamine, N1-(9-anthracenylmethyl)-N2-[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]- (CA INDEX NAME)

PAGE 1-A



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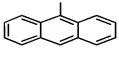
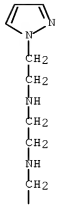


RN 1152004-07-3 HCAPLUS
CN 1,2-Ethanediamine, N1-(9-anthracenylmethyl)-N2-[2-(1H-pyrazol-1-yl)ethyl]- (CA INDEX NAME)

PAGE 1-A



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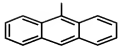
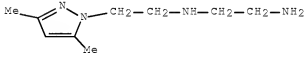
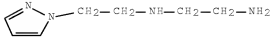


IT 511513-23-8 782501-70-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant for preparation of substituted pyrazolyldiamine)
RN 511513-23-8 HCAPLUS
CN 1,2-Ethanediamine, N1-[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]- (CA INDEX NAME)



RN 782501-70-6 HCAPLUS
CN 1,2-Ethanediamine, N1-[2-(1H-pyrazol-1-yl)ethyl]- (CA INDEX NAME)

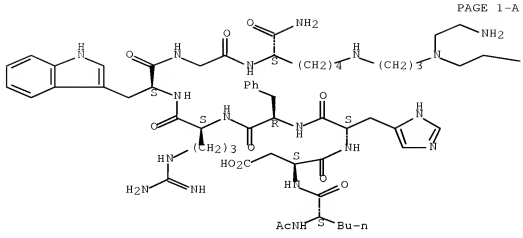


REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

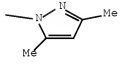
L49 ANSWER 3 OF 21 HCAPLUS COPYRIGHT 2009 ACS on STN DUPLICATE 3
ACCESSION NUMBER: 2007:1476534 HCAPLUS Full-text
DOCUMENT NUMBER: 149:241344
TITLE: A 99mTc(CO)3-labeled pyrazolyl-α-melanocyte-stimulating hormone analog conjugate for melanoma targeting
AUTHOR(S): Raposinho, Paula D.; Correia, Joao D. G.; Alves, Susana; Botelho, Maria F.; Santos, Ana C.; Santos, Isabel
CORPORATE SOURCE: Departamento de Quimica, ITN, Sacavem, 2686-953, Port.
SOURCE: Nuclear Medicine and Biology (2008), 35(1), 91-99 CODEN: NMBIEO; ISSN: 0969-8051
PUBLISHER: Elsevier Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 28 Dec 2007
AB Melanoma primary tumors can be, in most cases, removed surgically, whereas there is no satisfactory treatment for metastatic melanoma, being almost always lethal at this stage. Therefore, early detection of primary melanoma tumors is essential. The finding that melanocortin-1 receptor (MC1R) is overexpressed in isolated melanoma cells and melanoma tissues led to the radiolabeling of several α-MSH (α-MSH) analogs for early detection and treatment of melanoma. We have coupled the α-MSH analog Ac-Nle-Asp-His-D-Phe-Arg-Trp-Gly-Lys-NH2, through the ε-amino group of Lys11, to a pyrazolyl-containing chelator (pz). The resulting pz-α-MSH analog reacted with the fac-[99mTc(CO)3]+ moiety, giving [Ac-Nle4,Asp5,D-Phe7,Lys11(pz- 99mTc(CO)3)]α-MSH4-11 in high yield, high specific activity and high radiochem. purity. This radioconjugate, which presents remarkable stability in vitro, exhibited time- and temperature-dependent internalization (4 h at 37°C; 56.7% maximum internalization) and high cellular retention (only 38% was released from the cell after 5 h) in murine melanoma B16F1 cells. A significant tumor uptake [4.2 ± 0.9%ID/g, at 4 h postinjection (p.i.)] was also obtained in melanoma-bearing C57BL6 mice. The in vivo affinity and specificity of the radioconjugate to MC1R were demonstrated by receptor-blocking studies with the potent NDP-MSH agonist (63.5% reduction in tumor uptake at 4 h p.i.).
CC 8-9 (Radiation Biochemistry)
IT 163932-31-8 1044531-54-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(99mTc(CO)3-labeled pyrazolyl-α-MSH analog conjugate for melanoma imaging)
IT 1044531-54-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(99mTc(CO)3-labeled pyrazolyl-α-MSH analog conjugate for melanoma imaging)
RN 1044531-54-5 HCAPLUS
CN L-Lysinamide, N-acetyl-L-norleucyl-L-α-aspartyl-L-histidyl-D-phenylalanyl-L-arginyl-L-tryptophylglycyl-N6-[3-[(2-aminoethyl)[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]propyl]- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 4 OF 21 HCAPLUS COPYRIGHT 2009 ACS on STN DUPLICATE 4
ACCESSION NUMBER: 2007:159588 HCAPLUS Full-text
DOCUMENT NUMBER: 146:413668
TITLE: Evaluation of two chelators for labeling a PNA monomer with the fac-[99mTc(CO)3]+ moiety
AUTHOR(S): Xavier, Catarina; Pak, Jae-Kyoung; Santos, Isabel; Alberto, Roger
CORPORATE SOURCE: Departamento de Quimica, Instituto Tecnologico e Nuclear, Estrada Nacional 10, Sacavem, 2686-953, Port.
SOURCE: Journal of Organometallic Chemistry (2007), 692(6), 1332-1339
CODEN: JORCAI; ISSN: 0022-328X
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:413668
ED Entered STN: 13 Feb 2007
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB A PNA monomer containing thymine as nucleobase was synthesized, characterized and coupled to the pyrazolyl containing ligand 3,5-Me2pz(CH2)2N((CH2)3COOH)(CH2)2NHBoc and to a modified cysteine S-(carboxymethyl-pentafluorophenyl)-N-[(trifluoro)carbonyl]-cysteine Me ester yielding the bifunctional chelators I and II, resp. Reactions of I and II with the Re(I) tricarbonyl starting material [Re(CO)3(H2O)3]Br afforded the complexes fac-[Re(CO)3(κ3-I)]+ and fac-[Re(CO)3(κ3-II)], resp. The identities of the rhenium complexes have been established based on IR spectroscopy, elemental anal., ESI-MS spectrometry and HPLC. The multinuclear NMR spectroscopy (1H, 13C, g-COSY, g-HSQC) has also been very informative in the case of complex fac-[Re(CO)3(κ3-I)]+, showing the presence of rotamers in solution For fac-[Re(CO)3(κ3-II)] the NMR spectrum was too complex due to the presence of rotamers and diastereoisomers. The radioactive congeners of the rhenium complexes, fac-[99mTc(CO)3(κ3-6)]+ and fac-[99mTc(CO)3(κ3-7)], have been prepared by reacting the precursor fac-[99mTc(CO)3(H2O)3]+ with the corresponding ligands and their identities were established by comparing their HPLC chromatograms with those of the rhenium analogs.

CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 26

ST pyrazolyl deriv thyminyl glycinate chelator prepn complexation rhenium technetium; cysteinyl deriv thyminyl glycinate chelator prepn complexation rhenium technetium; rhenium thyminyl glycinate pyrazolyl cysteinyl deriv carbonyl complex prepn; technetium thyminyl glycinate pyrazolyl cysteinyl deriv carbonyl complex prepn; peptide nucleic acid monomer thymine deriv prepn coupling

IT Transition metal complexes
RL: SPN (Synthetic preparation); PREP (Preparation)
(cysteine-containing peptide; preparation of pyrazolyl-/cysteinyl-containing thyminyl glycinate derivative bifunctional chelators and their rhenium/technetium carbonyl complexes)

IT Peptides, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(cysteine-containing, transition metal complexes; preparation of pyrazolyl-/cysteinyl-containing thyminyl glycinate derivative bifunctional chelators and their rhenium/technetium carbonyl complexes)

IT Transition metal complexes
RL: SPN (Synthetic preparation); PREP (Preparation)
(peptide; preparation of pyrazolyl-/cysteinyl-containing thyminyl glycinate derivative bifunctional chelators and their rhenium/technetium carbonyl complexes)

IT Peptide nucleic acids
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrazolyl-/cysteinyl-containing thyminyl glycinate derivative bifunctional chelators and their rhenium/technetium carbonyl complexes)

IT Peptides, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(transition metal complexes; preparation of pyrazolyl-/cysteinyl-containing thyminyl glycinate derivative bifunctional chelators and their rhenium/technetium carbonyl complexes)

IT 5292-43-3, tert-Butylbromoacetate 14533-84-7 20924-05-4, Thymin-1-ylacetic acid 55757-46-5, N-(tert-Butoxycarbonyl)-L-cysteine methyl ester 128421-86-3 163932-31-8 782501-78-4 828915-71-5

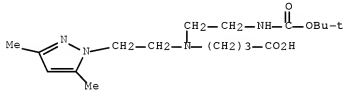
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyrazolyl-/cysteinyl-containing thyminyl glycinate derivative
bifunctional chelators and their rhenium/technetium carbonyl complexes)

IT 24997-00-0P 152774-08-8P 933789-23-2P 933789-24-3P
933789-25-4P 933789-27-6P 933789-33-4P 1005462-11-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrazolyl-/cysteinyl-containing thyminyl glycinate derivative
bifunctional chelators and their rhenium/technetium carbonyl complexes)

IT 933789-29-8P 933789-32-3P 933789-34-5P 933789-35-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of pyrazolyl-/cysteinyl-containing thyminyl glycinate derivative
bifunctional chelators and their rhenium/technetium carbonyl complexes)

IT 782501-78-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyrazolyl-/cysteinyl-containing thyminyl glycinate derivative
bifunctional chelators and their rhenium/technetium carbonyl complexes)

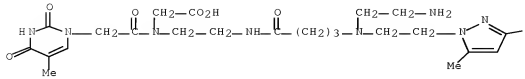
RN 782501-78-4 HCAPLUS
CN Butanoic acid, 4-[[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl][2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]- (CA INDEX NAME)



IT 933789-25-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrazolyl-/cysteinyl-containing thyminyl glycinate derivative
bifunctional chelators and their rhenium/technetium carbonyl complexes)

RN 933789-25-4 HCAPLUS
CN Glycine, N-[2-[[4-[(2-aminoethyl)[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]-1-oxobutyl]amino]ethyl]-N-[2-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]- (CA INDEX NAME)

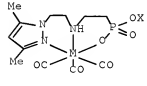
PAGE 1-A



PAGE 1-B

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 5 OF 21 HCAPLUS COPYRIGHT 2009 ACS on STN DUPLICATE 5
ACCESSION NUMBER: 2008:220414 HCAPLUS Full-text
DOCUMENT NUMBER: 150:121723
TITLE: A pyrazolylamine-phosphonate monoester chelator for the fac-[M(CO)3]+ core (M = Re, 99mTc): synthesis, coordination properties and biological assessment
AUTHOR(S): Palma, Elisa; Oliveira, Bruno L.; Figueira, Flavio; Correia, Joao D. G.; Raposinho, Paula D.; Santos, Isabel
CORPORATE SOURCE: Departamento de Quimica, ITN, Sacavem, 2686-953, Port.
SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (2007), 50(13), 1176-1184
CODEN: JLCRD4; ISSN: 0362-4803
PUBLISHER: John Wiley & Sons Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 21 Feb 2008
GI



I

AB Rhenium and technetium tricarbonyl pyrazolyl phosphonates I (6, 6a; M = Re, 99mTc; X = Et) were prepared as radioimaging or radiotherapeutic agents and probed for biodistribution and biostability in a number of mice organs. Aiming to develop new strategies for the labeling of hydroxyl-containing biomols. with the organometallic core fac-[99mTc(CO)3]+, a new model bifunctional chelator, Et hydrogen (2-{[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino}ethyl)phosphonate (L4), combining a pyrazolyl-amine chelating

group and a monophosphonate Et ester function (-P(O)OHOEt). The phosphonate group allows metal stabilization, and, simultaneously, can be considered as a potential attachment site for a biomol. Reaction of L4 with the precursor [99mTc(H2O)3(CO)3]+ gave the model radiocomplex I, [99mTc(CO)3(k3-L4)] (6a). This radiocomplex was identified by comparing its chromatog. profile with that of the corresponding Re analog 6. Radiocomplex 6a is moderately lipophilic (log Po/w = 1.07), presenting high stability in vitro without any measurable decomposition or ligand exchange, even in the presence of strong competing chelators such as histidine and cysteine at 37° for 24 h. Biodistribution studies of the complex in CD-1 mice indicated a rapid blood clearance, and a rapid clearance from main organs, occurring primarily through the hepatobiliary pathway. Complex 6a presents also a high robustness in vivo, demonstrated by its resistance to metabolic degradation in blood, and intact excretion into the urine, after RP-HPLC anal. of blood and urine samples. Hydrolyzed forms of I (X = H) can be coupled with hydroxyl-containing biomols. as a phosphonate ester, thus allowing radioactive labeling.

CC 29-7 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 63, 78

ST technetium rhenium chelate pyrazolyl aminophosphonate prepn
biodistribution biostability; radioactive labeling agent prepn technetium chelate tricarbonyl pyrazolyl aminophosphonate; pharmacokinetics
radioactive labeling agent technetium chelate tricarbonyl pyrazolyl aminophosphonate

IT Chelates
RL: PKT (Pharmacokinetics); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(conjugates, technetium, rhenium; preparation, biodistribution and biostability of rhenium and technetium-99m tricarbonyl pyrazolyl aminophosphonate chelates as radioimaging and radiotherapy agents)

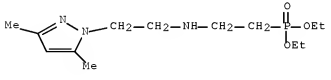
IT Partition
(octanol-water; preparation, biodistribution and biostability of rhenium and technetium-99m tricarbonyl pyrazolyl aminophosphonate chelates as radioimaging and radiotherapy agents)

IT Bioavailability
Chelating agents
Isotope indicators
Lipophilicity
Pharmacokinetics
Radiography
Radiotherapy
(preparation, biodistribution and biostability of rhenium and technetium-99m tricarbonyl pyrazolyl aminophosphonate chelates as radioimaging and radiotherapy agents)

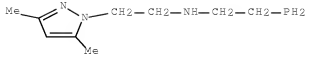
IT Group VIIB element complexes
RL: PKT (Pharmacokinetics); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation, biodistribution and biostability of rhenium and technetium-99m tricarbonyl pyrazolyl aminophosphonate chelates as radioimaging and radiotherapy agents)

IT Chelates
Phosphonates
RL: PKT (Pharmacokinetics); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(technetium, rhenium; preparation, biodistribution and biostability of rhenium and technetium-99m tricarbonyl pyrazolyl aminophosphonate chelates as radioimaging and radiotherapy agents)

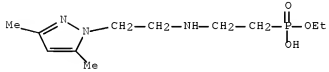
IT 5324-30-1, Phosphonic acid, 2-bromoethyl-, diethyl ester 67000-35-5
524744-56-7 828915-71-5, Rhenium(1+), triaquatricarbonyl-, bromide
(OC-6-22)-
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation, biodistribution and biostability of rhenium and technetium-99m
tricarbonyl pyrazolyl aminophosphonate chelates as
radioimaging and radiotherapy agents)
IT 62821-88-9P 144369-80-2P 1096702-45-2P 1096702-46-3P
1096702-50-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation, biodistribution and biostability of rhenium and technetium-99m
tricarbonyl pyrazolyl aminophosphonate chelates as
radioimaging and radiotherapy agents)
IT 1096702-47-4P 1096702-48-5P 1097641-45-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, biodistribution and biostability of rhenium and technetium-99m
tricarbonyl pyrazolyl aminophosphonate chelates as
radioimaging and radiotherapy agents)
IT 1096702-49-6P
RL: BSU (Biological study, unclassified); PKT (Pharmacokinetics); SPN
(Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(99mTc complex; preparation, biodistribution and biostability of rhenium and
technetium-99m tricarbonyl pyrazolyl aminophosphonate chelates
as radioimaging and radiotherapy agents)
IT 1096702-45-2P 1096702-46-3P 1096702-50-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation, biodistribution and biostability of rhenium and technetium-99m
tricarbonyl pyrazolyl aminophosphonate chelates as
radioimaging and radiotherapy agents)
RN 1096702-45-2 HCAPLUS
CN Phosphonic acid, P-[2-[[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]ethyl]-
, diethyl ester (CA INDEX NAME)



RN 1096702-46-3 HCAPLUS
CN 1H-Pyrazole-1-ethanamine, 3,5-dimethyl-N-(2-phosphinoethyl)- (CA INDEX
NAME)



RN 1096702-50-9 HCAPLUS
CN Phosphonic acid, P-[2-[[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]ethyl]-, monoethyl ester (CA INDEX NAME)



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 6 OF 21 HCAPLUS COPYRIGHT 2009 ACS on STN DUPLICATE 6
ACCESSION NUMBER: 2007:22645 HCAPLUS Full-text
DOCUMENT NUMBER: 146:307704
TITLE: Rhenium(V) oxocomplexes with novel pyrazolyl-based N4- and N3S-donor chelators
AUTHOR(S): Moura, Carolina; Vitor, Rute F.; Maria, Leonor; Paulo, Antonio; Santos, Isabel C.; Santos, Isabel
CORPORATE SOURCE: Departamento de Quimica, ITN, Sacavem, 2686-953, Port.
SOURCE: Dalton Transactions (2006), (47), 5630-5640
CODEN: DTARAF; ISSN: 1477-9226
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:307704
ED Entered STN: 08 Jan 2007
AB The novel pyrazolyl-based ligands 3,5-Me2pz(CH2)2NH(CH2)2NH(CH2)2NH2 (1) and pz*(CH2)2NH-Gly-CH2STrit (pz* = pz (8), 3,5-Me2pz (9), 4-(EtOOC)CH2-3,5-Me2pz (10)) were synthesized, and their suitability to stabilize Re(V) oxocomplexes was evaluated using different starting materials, (NBu4)[ReOCl4], [ReOCl3(PPh3)2] and trans-[ReO2(py)4]Cl. Compound 1 reacts with trans-[ReO2(py)4]Cl yielding the cationic compound [ReO(OMe){3,5-Me2pz(CH2)2N(CH2)2NH(CH2)2NH2}](BPh4) (11) in a low isolated yield. In contrast, the neutral complexes [ReO{pz*(CH2)2NH-Gly-CH2S}] (pz* = pz (12), 3,5-Me2pz (13), 4-(EtOOCCH2)-3,5-Me2pz (14)) were synthesized almost quant. by reacting [ReOCl3(PPh3)2] or (NBu4)[ReOCl4] with the trityl-protected chelators 8-10. The x-ray diffraction anal. of 11 and 13 confirmed the tetradentate coordination mode of the resp. ancillary ligands. In 11 the monoanionic chelator coordinates to the metal through four N atoms, while in 13 the chelator is trianionic, coordinating to the metal through three nitrogens and one S atom. Solution NMR studies of 12-14, including two-dimensional NMR techniques (1H COSY and 1H/13C HSQC), confirmed that the N3S coordination mode of the chelators is retained in solution Unlike 11, complexes 12-14 may be considered relevant in the development of radiopharmaceuticals, as further

corroborated by the synthesis of the congener [99mTcO(pz(CH2)2-NH-Gly-CH2S)] (12a). This radioactive compound was obtained from 99mTcO4- in aqueous medium, in almost quant. yield and with high specific activity and radiochem. purity.

CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 8, 75

IT Crystal structure
Molecular structure
(of oxorhenium pyrazolyl-based N4- and N3S-donor chelating ligand complexes)

IT 927883-68-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(for preparation of pyrazolyl-based N3S-donor chelating ligand and its oxorhenium complex)

IT 302-01-2, Hydrazine, reactions 1074-82-4, Potassium phthalimide 1972-28-7, Diethylazodicarboxylate 7087-68-5, DIPEA 67000-35-5 91425-33-1 119291-22-4 927883-81-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of pyrazolyl-based N3S-donor chelating ligand and its oxorhenium complexes)

IT 62821-88-9P 101395-71-5P, 1H-Pyrazole-1-ethanamine 121751-71-1P 144369-80-2P 927883-67-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(for preparation of pyrazolyl-based N3S-donor chelating ligand and its oxorhenium complexes)

IT 67000-34-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of pyrazolyl-based N4-chelating ligand and its oxorhenium complexes)

IT 383-63-1P, Ethyl trifluoroacetate
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(for preparation of pyrazolyl-based N4-donor chelating ligand and its oxorhenium complexes)

IT 111-40-0 24424-99-5, Di-tert-butyl dicarbonate 120131-72-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of pyrazolyl-based N4-donor chelating ligand and its oxorhenium complexes)

IT 53675-30-2, Tetrabutylammonium tetrachlorooxorhenate
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of rhenium oxo pyrazolyl-based N3S-donor chelating ligand complex)

IT 17442-18-1, Trichloro(oxo)bis(triphenylphosphine)rhenium
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of rhenium oxo pyrazolyl-based N3S-donor chelating ligand complexes)

IT 31429-86-4, trans-[Dioxotetrakis(pyridine)]rhenium(1+) chloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of rhenium oxo pyrazolyl-based N4-donor chelating ligand complex)

IT 23288-60-0, Sodium tetraoxotechnetate(1-)-99Tc
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of technetium-99m pyrazolyl-based N4-donor chelating ligand complex)

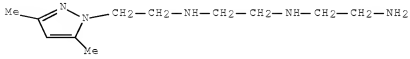
IT 927883-66-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with dioxorhenium pyridine complex)

IT 927883-66-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with dioxorhenium pyridine complex)

RN 927883-66-7 HCAPLUS

CN 1,2-Ethanediamine, N1-(2-aminoethyl)-N2-[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]- (CA INDEX NAME)



REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 7 OF 21 HCAPLUS COPYRIGHT 2009 ACS on STN DUPLICATE 7

ACCESSION NUMBER: 2006:711846 HCAPLUS Full-text

DOCUMENT NUMBER: 146:223509

TITLE: Pyrazolyl conjugates of bombesin: A new tridentate ligand framework for the stabilization of fac-[M(CO)3]+ moiety

AUTHOR(S): Alves, Susana; Correia, Joao D. G. ; Santos, Isabel; Veerendra, Bhadrasetty; Sieckman, Gary L.; Hoffman, Timothy J.; Rold, Tammy L.; Figueroa, Said Daibes; Retzloff, Lauren; McCrate, Joseph; Prasanphanich, Adam; Smith, Charles J.

CORPORATE SOURCE: Department of Radiology, University of Missouri-Columbia School of Medicine, Columbia, MO, 65211, USA

SOURCE: Nuclear Medicine and Biology (2006), 33(5), 625-634 CODEN: NMBIEO; ISSN: 0969-8051

PUBLISHER: Elsevier Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 21 Jul 2006

AB We have described the synthesis of tridentate pyrazolyl ligand frameworks for coordination to the fac-[*M(CO)3]+ metal fragment (*M = 186/188Re or 99mTc). These ligands impart a degree of kinetic inertness on the metal center, warranting their study in biol. systems. We herein report in vitro/in vivo radiolabeling investigations of a new series of pyrazolyl bombesin (BBN) conjugates radiolabeled via the Isolink kit. These new conjugates are based on the general structure [99mTc-pyrazolyl-X-BBN[7-14]NH2], where X = β-alanine, serylserylserine or glycylglycylglycine. The pyrazolyl ligand is a tridentate ligand framework that coordinates the metal center through nitrogen donor atoms. The results of these investigations demonstrate the ability of these new conjugates to specifically target the gastrin-releasing peptide receptor subtype 2, which is overexpressed on human prostate PC-3 cancerous tissues. Therefore, these studies suggest the tridentate pyrazolyl ligand framework to be an ideal candidate for the design and development of low-valent 99mTc-based diagnostic radiopharmaceuticals based on BBN or other targeting vectors.

CC 8-9 (Radiation Biochemistry)

IT 163932-31-8 924660-90-2 924660-91-3 924660-92-4
RL: RCT (Reactant); RACT (Reactant or reagent)

(pyrazolyl conjugates of bombesin: new tridentate ligand framework for stabilization of fac-[M(CO)3]+ moiety)

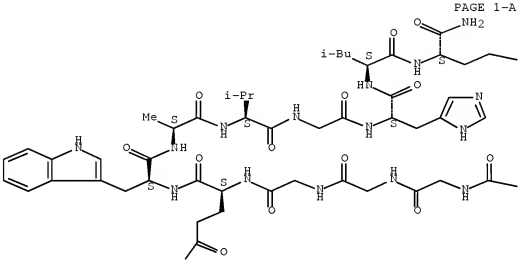
IT 924660-90-2 924660-91-3 924660-92-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(pyrazolyl conjugates of bombesin: new tridentate ligand framework for stabilization of fac-[M(CO)3]+ moiety)

RN 924660-90-2 HCAPLUS

CN L-Methioninamide, N-[4-[(2-aminoethyl)[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]-1-oxobutyl]glycylglycylglycyl-L-glutaminyl-L-tryptophyl-L-alanyl-L-valylglycyl-L-histidyl-L-leucyl- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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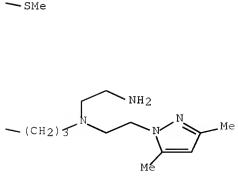
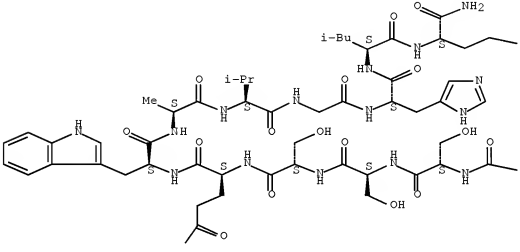


PAGE 2-A

RN 924660-91-3 HCAPLUS
CN L-Methioninamide, N-[4-[(2-aminoethyl)[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]-1-oxobutyl]-L-seryl-L-seryl-L-seryl-L-glutaminyl-L-tryptophyl-L-alanyl-L-valylglycyl-L-histidyl-L-leucyl- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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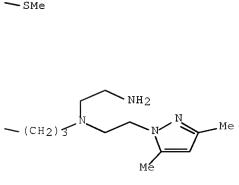
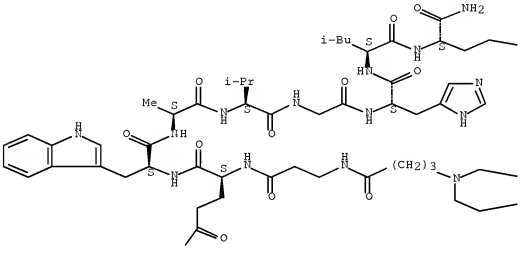


PAGE 2-A

RN 924660-92-4 HCAPLUS
CN L-Methioninamide, N-[4-[(2-aminoethyl)[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]-1-oxobutyl]-β-alanyl-L-glutaminyl-L-tryptophyl-L-alanyl-L-valylglycyl-L-histidyl-L-leucyl- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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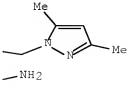

H2N

REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 8 OF 21 HCAPLUS COPYRIGHT 2009 ACS on STN DUPLICATE 8
ACCESSION NUMBER: 2005:205084 HCAPLUS Full-text
DOCUMENT NUMBER: 142:406796
TITLE: Pyrazolyl Derivatives as Bifunctional Chelators for Labeling Tumor-Seeking Peptides with the fac-[M(CO)3]+ Moiety (M = 99mTc, Re): Synthesis, Characterization, and Biological Behavior
AUTHOR(S): Alves, Susana; Paulo, Antonio; Correia, Joao D. G.; Gano, Lurdes; Smith, Charles J.; Hoffman, Timothy J.; Santos, Isabel
CORPORATE SOURCE: Departamento de Quimica, ITN, Sacavem, 2686-953, Port.
SOURCE: Bioconjugate Chemistry (2005), 16(2), 438-449
CODEN: BCCHES; ISSN: 1043-1802
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 09 Mar 2005
AB Radiolabeling of biol. active mols. with the [99mTc(CO)3]+ unit has been of primary interest in recent years. With this in mind, we herein report sym. (L1) and asym. (L2-L5) pyrazolyl-containing chelators that have been evaluated in radiochem. reactions with the synthon [99mTc(H2O)3(CO)3]+ (1a). These reactions yielded the radioactive building blocks [99mTc(CO)3(k3-L)]+ (L = L1-L5, 2a-6a), which were identified by RP-HPLC. The corresponding Re surrogates (2-6) allowed for macroscopic identification of the radiochem. conjugates. Complexes 2a-6a, with log Po/w values ranging from -2.35 to 0.87, were obtained in yields of ≥90% using ligand concns. in the 10-5-10-4 M range. Challenge studies with cysteine and histidine revealed high stability for all of these radioactive complexes, and biodistribution studies in mice indicated a fast rate of blood clearance and high rate of total radioactivity excretion, occurring primarily through the renal-urinary pathway. Based on the framework of the asym. chelators, the novel bifunctional ligands 3,5-Me2-pz(CH2)2N((CH2)3COOH)(CH2)2NH2 (L6) and pz(CH2)2N((CH2)3COOH)(CH2)2NH2 (L7) have been synthesized and their coordination chemical toward (NEt4)2[ReBr3(CO)3] (1) has been explored. The resulting complexes, fac-[Re(CO)3(k3-L)]Br (L6 (7), L7 (8)), contain tridentate ancillary ligands that are coordinated to the metal center through the pyrazolyl and amine nitrogen atoms, as observed for the other related building blocks. L6 and L7 were coupled to a glycylglycine Et ester dipeptide, and the resulting functionalized ligands were used to prepare the model complexes fac-[Re(CO)3(κ3-3,5-Me2- pz(CH2)2N(glygly)(CH2)2NH2)]+ (9/9a) and fac-[Re(CO)3(κ3-pz(CH2)2N(CH2)3(glygly)(CH2)2NH2)]+ (10/10a) (M = Re, 99mTc). These small conjugates have been fully characterized and are reported herein. On the basis of the in vitro/in vivo behavior of the model complexes (2a-6a, 9a, 10a), we chose to evaluate the in vitro/in vivo biol. behavior of a new tumor-seeking Bombesin pyrazolyl conjugate, [(L6)-G-G-G-Q-W-A-V-G-H-L-M-NH2], that has been labeled with the [99mTc(CO)3]+ metal fragment. Stability, in vitro cell binding assays, and pharmacokinetics studies in normal mice are reported herein.
CC 8-9 (Radiation Biochemistry)

Section cross-reference(s): 63, 78

ST pyrazolyl bifunctional chelator technetium 99m prepn biodistribution; rhenium pyrazolyl complex prepn

IT Drug delivery systems
(carriers; pyrazolyl derivs. as bifunctional chelators for labeling tumor-seeking peptides with 99mTc or Re)

IT Human
Imaging agents
Neoplasm
Prostate gland, neoplasm
Radiopharmaceuticals
(pyrazolyl derivs. as bifunctional chelators for labeling tumor-seeking peptides with 99mTc or Re)

IT 795271-47-5P 796031-75-9P 850494-15-4P 850494-16-5P 850494-17-6P 850494-18-7P 850494-19-8P 850494-21-2P 850494-22-3P
RL: DGN (Diagnostic use); PKT (Pharmacokinetics); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(pyrazolyl derivs. as bifunctional chelators for labeling tumor-seeking peptides with 99mTc or Re)

IT 511513-19-2P 511513-21-6P 511513-22-7P 782501-83-1P 782501-84-2P 782501-85-3P 850494-14-3P 850494-20-1P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(pyrazolyl derivs. as bifunctional chelators for labeling tumor-seeking peptides with 99mTc or Re)

IT 107-15-3, Ethylenediamine, reactions 2087-41-4, Glycylglycine ethyl ester hydrochloride 2969-81-5, Ethyl 4-bromobutyrate 25908-22-9 119291-22-4, 1-(2-Bromoethyl)pyrazole 163932-31-8 511513-23-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(pyrazolyl derivs. as bifunctional chelators for labeling tumor-seeking peptides with 99mTc or Re)

IT 782501-70-6P 782501-71-7P 782501-72-8P 782501-76-2P 782501-77-3P 782501-78-4P 782501-79-5P 782501-80-8P 850480-64-7P 850480-65-8P 850480-66-9P 850480-67-0P 850480-68-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(pyrazolyl derivs. as bifunctional chelators for labeling tumor-seeking peptides with 99mTc or Re)

IT 511513-23-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(pyrazolyl derivs. as bifunctional chelators for labeling tumor-seeking peptides with 99mTc or Re)

RN 511513-23-8 HCAPLUS

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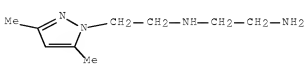

IT 782501-70-6P 782501-71-7P 782501-72-8P 782501-76-2P 782501-77-3P 782501-78-4P 782501-79-5P 782501-80-8P 850480-64-7P

850480-65-8P 850480-66-9P 850480-67-0P
850480-68-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(pyrazolyl derivs. as bifunctional chelators for labeling tumor-seeking peptides with 99mTc or Re)

RN 782501-70-6 HCAPLUS
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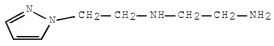

RN 782501-71-7 HCAPLUS
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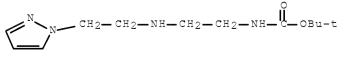

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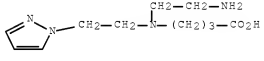

RN 782501-76-2 HCAPLUS
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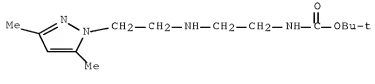

RN 782501-77-3 HCAPLUS
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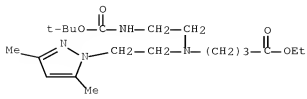
dimethyl-1H-pyrazol-1-yl)ethyl]amino]-, ethyl ester (CA INDEX NAME)



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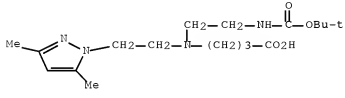
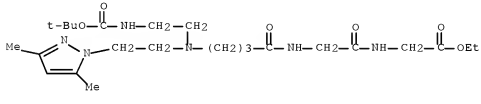


RN 782501-79-5 HCAPLUS
CN 2,5,10,13-Tetraazapentadecanedioic acid, 5-[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]-9,12-dioxo-, 1-(1,1-dimethylethyl) 15-ethyl ester (CA INDEX NAME)



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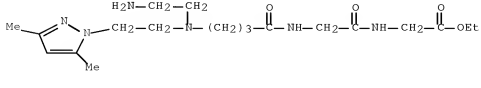

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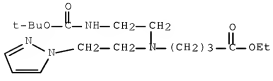

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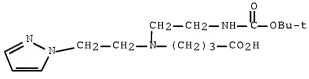

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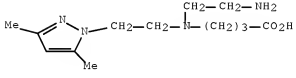
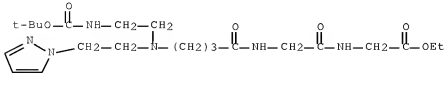
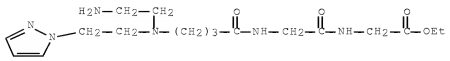


RN 850480-67-0 HCAPLUS
CN 2,5,10,13-Tetraazapentadecanedioic acid, 9,12-dioxo-5-[2-(1H-pyrazol-1-yl)ethyl]-, 1-(1,1-dimethylethyl) 15-ethyl ester (CA INDEX NAME)



RN 850480-68-1 HCAPLUS

CN Glycine, N-[4-[(2-aminoethyl)[2-(1H-pyrazol-1-yl)ethyl]amino]-1-oxobutyl]glycyl-, ethyl ester (CA INDEX NAME)



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 9 OF 21 HCAPLUS COPYRIGHT 2009 ACS on STN DUPLICATE 9
ACCESSION NUMBER: 2004:902222 HCAPLUS Full-text
DOCUMENT NUMBER: 141:387794
TITLE: Preparation of bifunctional pyrazole-containing tridentate ligands for rhenium and technetium tricarbonyl complexes
INVENTOR(S): Santos, Isabel R.; Galamba Correia, Joao D.; Rocha Paulo, Antonio M.; Alves, Susana; Vitor, Rute
PATENT ASSIGNEE(S): Mallinckrodt Inc., USA
SOURCE: PCT Int. Appl., 60 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004091669	A1	20041028	WO 2004-US11685	20040415
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CA 2522326	A1	20041028	CA 2004-2522326	20040415
EP 1644050	A1	20060412	EP 2004-759566	20040415
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JP 2007525452	T	20070906	JP 2006-510091	20040415
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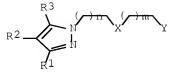
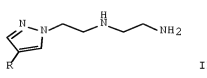
IN 2005CN02650	A	20070525	IN 2005-CN2650	20051014
NO 2005005334	A	20051111	NO 2005-5334	20051111
PRIORITY APPLN. INFO.:			EP 2003-76106 A	20030415

EP 2003-78217 A 20031010
WO 2004-US11685 W 20040415

OTHER SOURCE(S): MARPAT 141:387794
ED Entered STN: 28 Oct 2004
GI



I



II

AB The present invention relates to a chelating agent I [m = 0, 1; X = NR4, S; Y = SR5, NHR5, P(R5)2; R1, R3 = independently H, alkyl, aryl; R2 = H, CO2H, NHR6, (CH2)nCO2R6; R4 = H, alkyl, aryl, (CH2)nCO2R6, (CH2)nOR6; R5 = H, alkyl, aryl, (CH2)nCO2R6, (CH2)nOR6, R6 = H, alkyl, aryl; n = 1-10; when R1 = R3 = CH3, R2, R4, R5 are not all = H]. The invention further relates to a method and kit for the preparation of radiolabeled biomols. while using the chelating agent. Thus, pyrazole II (R = CO2H) was prepared by cyclocondensation of (OHC)2CHCO2Et with H2NNHCH2CH2OH, followed by tosylation and substitution with ethylenediamine and saponification Prepared compds. II (R = H, CO2H) underwent complexation with rhenium and technetium-99 to give the corresponding tricarbonyl complexes.

IC ICM A61K051-04
ICS C07D231-12; C07D231-14; A61P035-00

CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 9, 28

IT Chelating agents
(preparation of bifunctional pyrazole-containing tridentate ligands for rhenium and technetium tricarbonyl complexes)

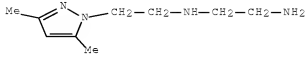
IT 60-24-2, 2-Mercaptoethanol 107-15-3, Ethylenediamine, reactions 109-84-2, (2-Hydroxyethyl)hydrazine 623-51-8, Ethyl 2-mercaptoacetate 2087-41-4, Glycylglycine ethyl ester hydrochloride 2969-81-5, Ethyl 4-bromobutyrate 67000-34-4 80370-42-9 119291-22-4, 1-(2-Bromoethyl)pyrazole 511513-23-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of bifunctional pyrazole-containing tridentate ligands for rhenium and technetium tricarbonyl complexes)

IT 487021-85-2P 782501-70-6P 782501-71-7P 782501-73-9P 782501-74-0P 782501-75-1P 782501-76-2P 782501-77-3P 782501-78-4P 782501-79-5P 782501-80-8P 782501-81-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of bifunctional pyrazole-containing tridentate ligands for rhenium and technetium tricarbonyl complexes)

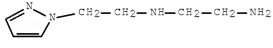
IT 782501-72-8P 782501-82-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of bifunctional pyrazole-containing tridentate ligands for rhenium and technetium tricarbonyl complexes)

IT 511513-23-8

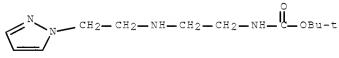
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of bifunctional pyrazole-containing tridentate ligands for rhenium
and technetium tricarbonyl complexes)
RN 511513-23-8 HCAPLUS
CN 1,2-Ethanediamine, N1-[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]- (CA INDEX NAME)



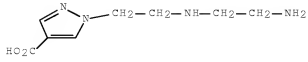
IT 782501-70-6P 782501-71-7P 782501-75-1P
782501-76-2P 782501-77-3P 782501-78-4P
782501-79-5P 782501-80-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of bifunctional pyrazole-containing tridentate ligands for rhenium
and technetium tricarbonyl complexes)
RN 782501-70-6 HCAPLUS
CN 1,2-Ethanediamine, N1-[2-(1H-pyrazol-1-yl)ethyl]- (CA INDEX NAME)



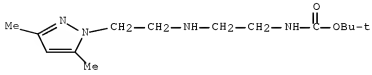
RN 782501-71-7 HCAPLUS
CN Carbamic acid, [2-[[2-(1H-pyrazol-1-yl)ethyl]amino]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



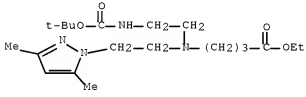
RN 782501-75-1 HCAPLUS
CN 1H-Pyrazole-4-carboxylic acid, 1-[2-[(2-aminoethyl)amino]ethyl]- (CA INDEX NAME)



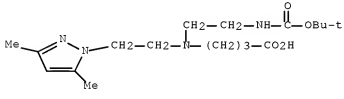
RN 782501-76-2 HCAPLUS
CN Carbamic acid, N-[2-[[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]ethyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



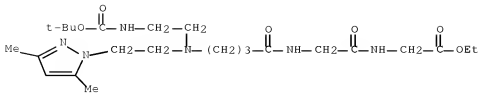
RN 782501-77-3 HCAPLUS
CN Butanoic acid, 4-[[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl][2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]-, ethyl ester (CA INDEX NAME)



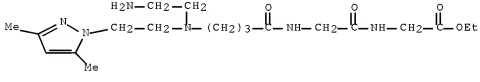
RN 782501-78-4 HCAPLUS
CN Butanoic acid, 4-[[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl][2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]- (CA INDEX NAME)



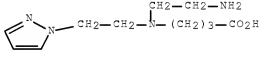
RN 782501-79-5 HCAPLUS
CN 2,5,10,13-Tetraazapentadecanedioic acid, 5-[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]-9,12-dioxo-, 1-(1,1-dimethylethyl) 15-ethyl ester (CA INDEX NAME)



RN 782501-80-8 HCAPLUS
CN Glycine, N-[4-[(2-aminoethyl)[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]-1-oxobutyl]glycyl-, ethyl ester (CA INDEX NAME)



IT 782501-72-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of bifunctional pyrazole-containing tridentate ligands for rhenium
and technetium tricarbonyl complexes)
RN 782501-72-8 HCAPLUS
CN Butanoic acid, 4-[(2-aminoethyl)[2-(1H-pyrazol-1-yl)ethyl]amino]- (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 10 OF 21 HCAPLUS COPYRIGHT 2009 ACS on STN DUPLICATE 10
ACCESSION NUMBER: 2004:1049014 HCAPLUS Full-text
DOCUMENT NUMBER: 142:168330
TITLE: Rhenium(I)- and technetium(I) tricarbonyl complexes anchored by bifunctional pyrazole-diamine and pyrazole-dithioether chelators
AUTHOR(S): Vitor, Rute F.; Alves, Susana; Correia, J. D. G.; Paulo, Antonio; Santos, Isabel
CORPORATE SOURCE: ITN, Estrada Nacional, Departamento de Quimica, Sacavem Codex, 2686-953, Port.
SOURCE: Journal of Organometallic Chemistry (2004), 689(25), 4764-4774
CODEN: JORCAI; ISSN: 0022-328X

PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:168330
ED Entered STN: 08 Dec 2004
AB The novel pyrazolyl containing ligands 4-(HOOC)pz(CH2)2NH(CH2)2NH2 (L1) and 4-(HOOCCH2)-3,5-Me2pz(CH2)2NH(CH2)2NH2 (L2), and 3,5-Me2pz(CH2)2S(CH2)2SCH2CH3 (L3), 3,5-Me2pz(CH2)2S(CH2)2SCH2COOEt (L4) and 3,5-Me2pz(CH2)2S(CH2)2SCH2COOH (L5) were synthesized, and their ability to stabilize complexes with the fac-[M(CO)3]+ (M = Re,99mTc) moiety was evaluated. Reactions of L1-L5 with (NEt4)2[Re(CO)3Br3] and/or [Re(CO)5Br] afforded complexes fac-[Re(CO)3(κ3-L)] (L = L1-L5 (1-5)), which contain the pyrazolyl ancillary ligands coordinated in a tridentate fashion. Complexes 1-5 were characterized by the common anal. techniques, which included single crystal x-ray diffraction anal. in the case of 4. The structural anal. of 4 confirmed the tridentate coordination mode of the pyrazole-dithioether ligand, which is facially coordinated to the Re(I) center through the N from the pyrazole ring and the two thioether S atoms, without involvement of the terminal ester functional group. The distorted octahedral coordination environment around the metal is completed by the three facial carbonyl ligands. The radioactive congeners of complexes 1, 3 and 4, fac-[99mTc(CO)3(κ3-L)]+ (L = L1 (1a), L3 (3a), L4 (4a)), were prepared by reacting the precursor fac-[99mTc(CO)3(H2O)3]+ with the corresponding ligands, and their identity confirmed by HPLC comparison with the Re surrogates. Complexes 1a and 3a were challenged in the presence of a large excess of histidine or cysteine, to evaluate their in vitro stability. Only a negligible displacement was observed, indicating that pyrazole-diamine and pyrazole-dithioether chelators provide a high kinetic inertness and/or stability to organometallic complexes with the fac-[99mTc(CO)3]+ moiety.
CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 28, 75
ST rhenium carbonyl pyrazole dithioether diamine chelator complex prepn; crystal structure rhenium carbonyl pyrazole dithioether chelator complex; stability in vitro technetium pyrazole dithioether chelator complex; technetium pyrazole dithioether diamine chelator complex prepn
IT Stability
(stability of technetium carbonyl pyrazole-thioether and -diamine chelator complexes in presence of histidine and cysteine)
IT 163932-31-8, fac-Triaquatricarbonyltechnetium(1+)-99Tc
RL: RCT (Reactant); RACT (Reactant or reagent)
(metastable; reactant for preparation of technetium carbonyl pyrazole-thioether and -diamine chelator complexes)
IT 827596-91-8P 827596-93-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and complexation with rhenium)
IT 782501-82-0P 827596-90-7P 827596-92-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and complexation with rhenium and technetium)
IT 782501-73-9P 827596-95-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactant for preparation of pyrazole-diamine chelator)
IT 827596-94-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactant for preparation of pyrazole-diamine chelators)
IT 782501-81-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactant for preparation of pyrazole-thioether chelators)

IT 1656-44-6, 2,4-Dinitrobenzenesulfonyl chloride 57260-73-8, N-tert-Butoxycarbonyl-1,2-ethanediamine 80370-42-9 503471-30-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant for preparation of pyrazole-diamine chelator)

IT 109-84-2, 2-Hydroxyethylhydrazine
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant for preparation of pyrazole-diamine chelators)

IT 75-08-1, Ethanethiol 623-51-8, Ethyl 2-mercaptoacetate 487021-85-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant for preparation of pyrazole-thioether chelators)

IT 14220-21-4, Bromopentacarbonylrhenium
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant for preparation of rhenium carbonyl pyrazole-diamine chelator complexes)

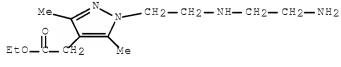
IT 25908-22-9, Bis(tetraethylammonium) tribromotricarbonylrhenate(2-)
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant for preparation of rhenium carbonyl pyrazole-thioether chelator complexes)

IT 52-90-4, L-Cysteine, processes 71-00-1, L-Histidine, processes
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PROC (Process)
(stability of technetium carbonyl pyrazole-thioether and -diamine chelator complexes in presence of)

IT 827596-91-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and complexation with rhenium)

RN 827596-91-8 HCAPLUS

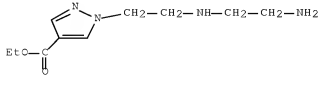
CN 1H-Pyrazole-4-acetic acid, 1-[2-[(2-aminoethyl)amino]ethyl]-3,5-dimethyl-, ethyl ester (CA INDEX NAME)



IT 827596-90-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and complexation with rhenium and technetium)

RN 827596-90-7 HCAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 1-[2-[(2-aminoethyl)amino]ethyl]-, ethyl ester (CA INDEX NAME)

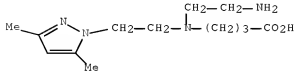


REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 11 OF 21 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:1487958 HCAPLUS Full-text
DOCUMENT NUMBER: 150:208111
TITLE: Re and 99m Tc organometallic complexes containing pendant L-arginine derivatives as potential probes of inducible nitric oxide synthase
AUTHOR(S): Oliveira, Bruno L.; Correia, Joao D. G.; Raposinho, Paula D.; Santos, Isabel; Ferreira, Antonio; Cordeiro, Carlos; Freire, Ana P.
CORPORATE SOURCE: Departamento de Quimica, ITN, Sacavem, 2686-953, Port.
SOURCE: Dalton Transactions (2009), (1), 152-162
CODEN: DTARAF; ISSN: 1477-9226
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 12 Dec 2008
AB Aiming to design radioactive compds. based on the core "99mTc(CO)3" for probing inducible nitric oxide synthase (iNOS) levels in vivo, we have synthesized conjugates containing a pyrazolyl-diamine chelating unit and pendant L-arginine analogs (substrates and inhibitors of NOS). Reaction of the conjugates with fac-[M(CO)3]+ (M = Re, 99m Tc) gave bioorganometallic complexes of the type fac-[M(CO)3(k3-L)] in good yield. After in vitro testing using the oxyHb NO capture assay, we concluded that the affinity of the inhibitor-containing conjugates to iNOS seems to be less affected upon metalation with rhenium than the substrate-containing conjugates. The complexes bearing guanidino substituted analogs of L-arginine still present considerable inhibitory action (Nω-monomethyl-L-arginine, Ki = 36 μM; Nω-nitro-L-arginine, Ki = 84 μM), being the first examples of organometallic complexes able to inhibit the iNOS. These results seem to indicate that 99mTc(CO)3-labeled L-arginine analogs, namely NOS inhibitors, may hold potential for monitoring increased levels of iNOS in vivo.
CC 7-3 (Enzymes)
Section cross-reference(s): 8, 9, 78
IT 74-79-3, L-Arginine, reactions 2577-94-8, L-Arginine methyl ester 6066-82-6, N-Hydroxysuccinimide 17035-90-4 25908-22-9, Bis(tetraethylammonium) fac-tribromotricarbonylrhenate(2-) 50903-99-6, Nω-Nitro-L-arginine methyl ester 163932-31-8, Fac-triaquatricarbonyltechnetium-99(1+) 850480-66-9 945384-90-7 1111224-57-7 1111224-64-6 1111224-73-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(Re and 99mTc organometallic complexes containing pendant L-arginine derivs. as potential probes of inducible nitric oxide synthase)
IT 1111224-18-0P 1111224-21-5P 1111224-23-7P 1111224-25-9P 1111224-29-3P 1111224-32-8P 1111224-35-1P 1111224-37-3P 1111224-40-8P 1111224-43-1P 1111224-46-4P 1111224-48-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(Re and 99mTc organometallic complexes containing pendant L-arginine derivs. as potential probes of inducible nitric oxide synthase)
IT 850480-66-9 1111224-57-7 1111224-64-6 1111224-73-7

RL: RCT (Reactant); RACT (Reactant or reagent)
(Re and 99mTc organometallic complexes containing pendant L-arginine derivs. as potential probes of inducible nitric oxide synthase)

RN 850480-66-9 HCAPLUS
CN Butanoic acid, 4-[(2-aminoethyl)[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]- (CA INDEX NAME)

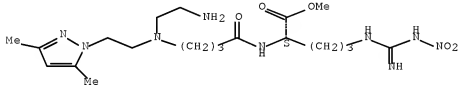


RN 1111224-57-7 HCAPLUS
CN L-Ornithine, N2-[4-[(2-aminoethyl)[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]-1-oxobutyl]-N5-[imino(nitroamino)methyl]-, methyl ester, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 1111224-40-8
CMF C20 H37 N9 O5

Absolute stereochemistry.



CM 2

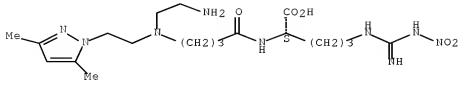
CRN 76-05-1
CMF C2 H F3 O2

RN 1111224-64-6 HCAPLUS
CN L-Ornithine, N2-[4-[(2-aminoethyl)[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]-1-oxobutyl]-N5-[imino(nitroamino)methyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 1111224-43-1
CMF C19 H35 N9 O5

Absolute stereochemistry.



CM 2

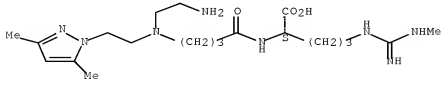
CRN 76-05-1
CMF C2 H F3 O2

RN 1111224-73-7 HCAPLUS
CN L-Ornithine, N2-[4-[(2-aminoethyl)[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]-1-oxobutyl]-N5-[imino(methylamino)methyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 1111224-48-6
CMF C20 H38 N8 O3

Absolute stereochemistry.

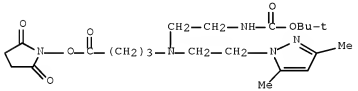


CM 2

CRN 76-05-1
CMF C2 H F3 O2

IT 1111224-18-0P 1111224-21-5P 1111224-23-7P
1111224-25-9P 1111224-29-3P 1111224-32-8P
1111224-35-1P 1111224-37-3P 1111224-40-8P
1111224-43-1P 1111224-46-4P 1111224-48-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(Re and 99mTc organometallic complexes containing pendant L-arginine derivs. as potential probes of inducible nitric oxide synthase)

RN 1111224-18-0 HCAPLUS
CN Butanoic acid, 4-[[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl][2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]-, 2,5-dioxo-1-pyrrolidinyl ester (CA INDEX NAME)

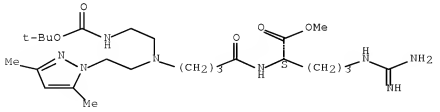


RN 1111224-21-5 HCAPLUS
CN 13-Oxa-3,8,11-triazapentadecanoic acid, 2-[3-[(aminoiminomethyl)amino]propyl]-8-[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]-14,14-dimethyl-4,12-dioxo-, methyl ester, (2S)-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 1111224-20-4
CMF C25 H46 N8 O5

Absolute stereochemistry.

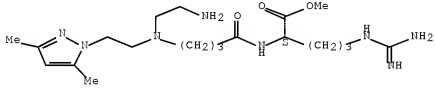


CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 1111224-23-7 HCAPLUS
CN L-Arginine, N2-[4-[(2-aminoethyl)[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]-1-oxobutyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.

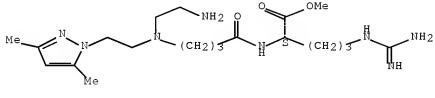


RN 1111224-25-9 HCAPLUS
CN L-Arginine, N2-[4-[(2-aminoethyl)[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]-1-oxobutyl]-, methyl ester, 2,2,2-trifluoroacetate (1:2) (CA INDEX NAME)

CM 1

CRN 1111224-23-7
CMF C20 H38 N8 O3

Absolute stereochemistry.



CM 2

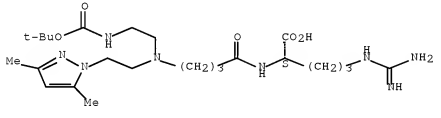
CRN 76-05-1
CMF C2 H F3 O2

RN 1111224-29-3 HCAPLUS
CN 13-Oxa-3,8,11-triazapentadecanoic acid, 2-[3-[(aminoiminomethyl)amino]propyl]-8-[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]-14,14-dimethyl-4,12-dioxo-, (2S)-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 1111224-28-2
CMF C24 H44 N8 O5

Absolute stereochemistry.

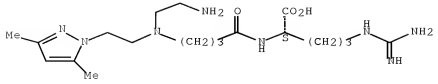


CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 1111224-32-8 HCAPLUS
CN L-Arginine, N2-[4-[(2-aminoethyl)[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]-1-oxobutyl]- (CA INDEX NAME)

Absolute stereochemistry.

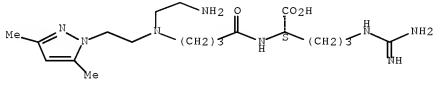


RN 1111224-35-1 HCAPLUS
CN L-Arginine, N2-[4-[(2-aminoethyl)[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]-1-oxobutyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 1111224-32-8
CMF C19 H36 N8 O3

Absolute stereochemistry.

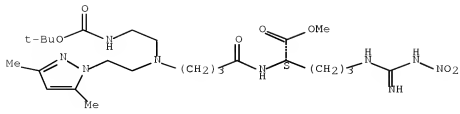


CM 2

CRN 76-05-1
CMF C2 H F3 O2

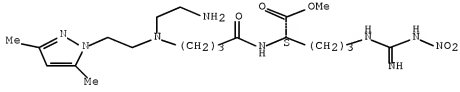
RN 1111224-37-3 HCAPLUS
CN 2,5,10,15-Tetraazahexadecanoic acid, 5-[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]-16-imino-11-(methoxycarbonyl)-16-(nitroamino)-9-oxo-, 1,1-dimethylethyl ester, (11S)- (CA INDEX NAME)

Absolute stereochemistry.



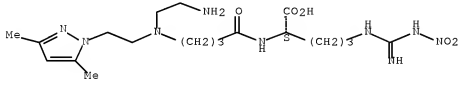
RN 1111224-40-8 HCAPLUS
CN L-Ornithine, N2-[4-[(2-aminoethyl)[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]-1-oxobutyl]-N5-[imino(nitroamino)methyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



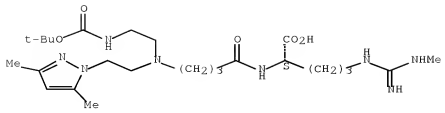
RN 1111224-43-1 HCAPLUS
CN L-Ornithine, N2-[4-[(2-aminoethyl)[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]-1-oxobutyl]-N5-[imino(nitroamino)methyl]- (CA INDEX NAME)

Absolute stereochemistry.



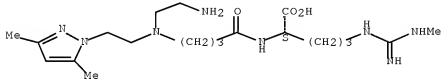
RN 1111224-46-4 HCAPLUS
CN 13-Oxa-3,8,11-triazapentadecanoic acid, 8-[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]-2-[3-[[imino(methylamino)methyl]amino]propyl]-14,14-dimethyl-4,12-dioxo-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 1111224-48-6 HCAPLUS
CN L-Ornithine, N2-[4-[(2-aminoethyl)[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]-1-oxobutyl]-N5-[imino(methylamino)methyl]- (CA INDEX NAME)

Absolute stereochemistry.

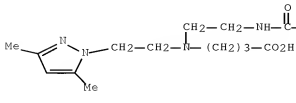


REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 12 OF 21 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:1206988 HCAPLUS Full-text
DOCUMENT NUMBER: 150:35664
TITLE: Synthesis, characterization, and evaluation of a novel 99mTc(CO)3 pyrazolyl conjugate of a peptide nucleic acid sequence. [Erratum to document cited in CA150:020350]
AUTHOR(S): Xavier, Catarina; Giannini, Clelia; Dall'Angelo, Sergio; Gano, Lurdes; Maiorana, Stefano; Alberto, Roger; Santos, Isabel
CORPORATE SOURCE: Departamento de Quimica, Instituto Tecnologico e Nuclear, Sacavem, 2686-953, Port.
SOURCE: JBIC, Journal of Biological Inorganic Chemistry (2008), 13(8), 1345
CODEN: JJBCFA; ISSN: 0949-8257
PUBLISHER: Springer GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 08 Oct 2008
AB On page 1335, in the author list, Sergio Dall'Angelo was omitted from the author list; the correct author list and author affiliations are given.
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 8, 78
IT Nucleic acid hybridization
(DNA-PNA; solid-phase preparation of peptide nucleic acid sequences, their conjugates with pyrazolyl chelator, and complexes with rhenium and 99-technetium (Erratum))
IT Imaging agents

(solid-phase preparation of peptide nucleic acid sequences, their conjugates
with pyrazolyl chelator, and complexes with rhenium and 99-technetium (Erratum))
IT Peptide nucleic acids
RL: BSU (Biological study, unclassified); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(solid-phase preparation of peptide nucleic acid sequences, their conjugates
with pyrazolyl chelator, and complexes with rhenium and 99-technetium (Erratum))
IT 1089234-29-6P
RL: BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(solid-phase preparation of peptide nucleic acid sequences, their conjugates
with pyrazolyl chelator, and complexes with rhenium and 99-technetium (Erratum))
IT 1089234-31-0 1089234-32-1
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(solid-phase preparation of peptide nucleic acid sequences, their conjugates
with pyrazolyl chelator, and complexes with rhenium and 99-technetium (Erratum))
IT 1089234-26-3P 1089234-28-5P
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(solid-phase preparation of peptide nucleic acid sequences, their conjugates
with pyrazolyl chelator, and complexes with rhenium and 99-technetium (Erratum))
IT 1089234-27-4P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(solid-phase preparation of peptide nucleic acid sequences, their conjugates
with pyrazolyl chelator, and complexes with rhenium and 99-technetium (Erratum))
IT 163932-31-8 782501-78-4 945384-90-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(solid-phase preparation of peptide nucleic acid sequences, their conjugates
with pyrazolyl chelator, and complexes with rhenium and 99-technetium (Erratum))
IT 1089234-30-9DP, resin-bound
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(solid-phase preparation of peptide nucleic acid sequences, their conjugates
with pyrazolyl chelator, and complexes with rhenium and 99-technetium (Erratum))
IT 782501-78-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(solid-phase preparation of peptide nucleic acid sequences, their conjugates
with pyrazolyl chelator, and complexes with rhenium and 99-technetium (Erratum))
RN 782501-78-4 HCAPLUS

CN Butanoic acid, 4-[[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl][2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]- (CA INDEX NAME)



L49 ANSWER 13 OF 21 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:462227 HCAPLUS Full-text
DOCUMENT NUMBER: 148:556216
TITLE: Melanoma targeting with α-melanocyte stimulating hormone analogs labeled with fac-[99mTc(CO)3]+: effect of cyclization on tumor-seeking properties
AUTHOR(S): Raposinho, Paula D.; Xavier, Catarina; Correia, Joao D. G.; Falcao, Soraia; Gomes, Paula; Santos, Isabel
CORPORATE SOURCE: Departamento de Quimica, ITN, Sacavem, 2686-953, Port.
SOURCE: JBIC, Journal of Biological Inorganic Chemistry (2008), 13(3), 449-459
CODEN: JJBCFA; ISSN: 0949-8257
PUBLISHER: Springer GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 15 Apr 2008
AB Early detection of primary melanoma tumors is essential because there is no effective treatment for metastatic melanoma. Several linear and cyclic radiolabeled α-MSH analogs have been proposed to target the melanocortin type 1 receptor (MC1R) overexpressed in melanoma. The compact structure of a rhenium-cyclized α-MSH analog (Re-CCMSH) significantly enhanced its in vivo tumor uptake and retention. Melanotan II (MT-II), a cyclic lactam analog of α-MSH (Ac-Nle-cyclo[Asp-His-DPhe-Arg-Trp-Lys]-NH2), is a very potent and stable agonist peptide largely used in the characterization of melanocortin receptors. Taking advantage of the superior biol. features associated with the MT-II cyclic peptide, the authors assessed the effect of lactam-based cyclization on the tumor-seeking properties of α-MSH analogs by comparing the pharmacokinetics profile of the 99mTc-labeled cyclic peptide βAla-Nle-cyclo[Asp-His-D-Phe-Arg-Trp-Lys]-NH2 with that of the linear analog βAla-Nle-Asp-His-DPhe-Arg-Trp-Lys-NH2 in melanoma-bearing mice. The authors have synthesized and coupled the linear and cyclic peptides to a bifunctional chelator containing a pyrazolyl-diamine backbone (pz) through the amino group of βAla, and the resulting pz-peptide conjugates were reacted with the fac-[99mTc(CO)3]+ moiety. The 99mTc(CO)3-labeled conjugates were obtained in high yield, high specific activity, and high radiochem. purity. The cyclic 99mTc(CO)3-labeled conjugate presents a remarkable internalization (87.1% of receptor-bound tracer and 50.5% of total applied activity, after 6 h at 37°) and cellular retention (only 24.7% released from the cells after 5 h) in murine melanoma B16F1 cells. A significant tumor uptake and retention was obtained in melanoma-bearing C57BL6 mice for the cyclic radioconjugate [9.26 ± 0.83 and 11.31 ± 1.83% ID/g at 1 and 4 h after injection, resp.]. The linear 99mTc(CO)3-pz-peptide presented lower values for both cellular internalization

and tumor uptake. Receptor blocking studies with the potent (Nle4,DPhe7)-αMSH agonist demonstrated the specificity of the radio-conjugates to MC1R (74.8% and 44.5% reduction of tumor uptake at 4 h after injection for cyclic and linear radio-conjugates, resp.).

CC 8-9 (Radiation Biochemistry)
Section cross-reference(s): 2, 14

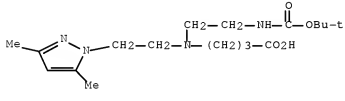
IT 524744-56-7 782501-78-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(melanoma targeting with α-MSH analogs labeled with fac-[99mTc(CO)3]+ and effect of cyclization on tumor-seeking properties)

IT 1025483-81-1P 1025483-83-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(melanoma targeting with α-MSH analogs labeled with fac-[99mTc(CO)3]+ and effect of cyclization on tumor-seeking properties)

IT 782501-78-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(melanoma targeting with α-MSH analogs labeled with fac-[99mTc(CO)3]+ and effect of cyclization on tumor-seeking properties)

RN 782501-78-4 HCAPLUS

CN Butanoic acid, 4-[[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl][2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]- (CA INDEX NAME)



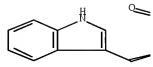
IT 1025483-81-1P 1025483-83-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(melanoma targeting with α-MSH analogs labeled with fac-[99mTc(CO)3]+ and effect of cyclization on tumor-seeking properties)

RN 1025483-81-1 HCAPLUS

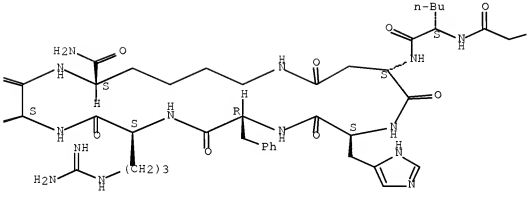
CN L-Lysinamide, N-[4-[(2-aminoethyl)[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]-1-oxobutyl]-β-alanyl-L-norleucyl-L-α-aspartyl-L-histidyl-D-phenylalanyl-L-arginyl-L-tryptophyl-, (3→8)-lactam (CA INDEX NAME)

Absolute stereochemistry.

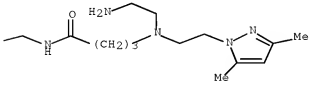
PAGE 1-A



PAGE 1-B



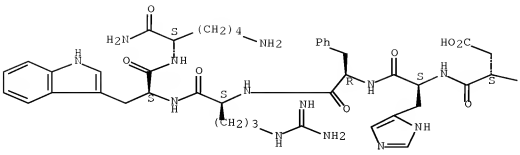
PAGE 1-C



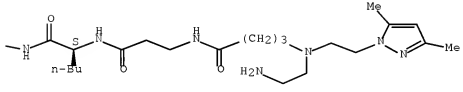
RN 1025483-83-3 HCAPLUS
CN L-Lysinamide, N-[4-[(2-aminoethyl)[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]-1-oxobutyl]-β-alanyl-L-norleucyl-L-α-aspartyl-L-histidyl-D-phenylalanyl-L-arginyl-L-tryptophyl- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

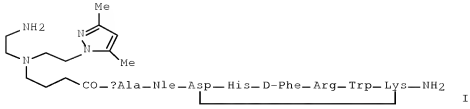


PAGE 1-B



REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 14 OF 21 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:1176860 HCAPLUS Full-text
DOCUMENT NUMBER: 149:576827
TITLE: Comparative Study of Chemical Approaches to the Solid-Phase Synthesis of a Tumor-Seeking α-MSH Analogue
AUTHOR(S): Valldosera, Magdalena; Monso, Marta; Xavier, Catarina; Raposinho, Paula; Correia, Joao D. G.; Santos, Isabel; Gomes, Paula
CORPORATE SOURCE: Departamento de Quimica, Faculdade de Ciencias (DQFCUP), Centro de Investigacao em Quimica da Universidade do Porto (CIQUP), Universidade do Porto, Oporto, 4169-007, Port.
SOURCE: International Journal of Peptide Research and Therapeutics (2008), 14(3), 273-281
CODEN: IJPRFC; ISSN: 1573-3149
PUBLISHER: Springer
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 01 Oct 2008
GI



I

AB The synthesis of a cyclic melanocortin analog I (H-pz-βAla-Nle-cyclo[Asp-His-DPhe-Arg-Trp-Lys]-NH2), where the Boc-protected derivative of a metal-chelating pyrazolyl ligand (pz) was inserted as an N-terminal residue, was accomplished by several different Fmoc/tBu and Boc/Bzl solid-phase strategies. On-resin cyclization was achieved immediately following incorporation of Asp, by condensation of the Asp side chain carboxyl with the Lys side chain primary amine after selective and simultaneous removal of side chain protecting groups. The success of the synthesis was highly dependent on the chemical strategy employed, with Boc/Bzl chemical giving the best results. On the light of these findings, Fmoc/tBu strategies are not advantageous for the solid-phase synthesis of this particular type of lactam-bridged peptides. Last, but not least, the target peptide was recently found to have promising tumor-seeking properties (J Biol Inorg Chem 13:449-459, 2008).

CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 2

IT 1025483-81-1P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(comparisons of solid-phase synthetic approaches to tumor-seeking α-MSH analog)

IT 81379-52-4 84624-27-1 109425-51-6 117014-32-1 146982-24-3 146982-27-6 167393-62-6 200336-86-3 204777-78-6, Fmoc-Lys(ivDde)-OH 269066-08-2 782501-78-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(comparisons of solid-phase synthetic approaches to tumor-seeking α-MSH analog)

IT 137668-62-3P 1084652-81-2P 1084652-83-4P 1084652-84-5P 1084652-87-8P 1084652-90-3P 1084652-93-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(comparisons of solid-phase synthetic approaches to tumor-seeking α-MSH analog)

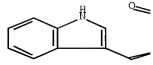
IT 1025483-81-1P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(comparisons of solid-phase synthetic approaches to tumor-seeking α-MSH analog)

RN 1025483-81-1 HCAPLUS

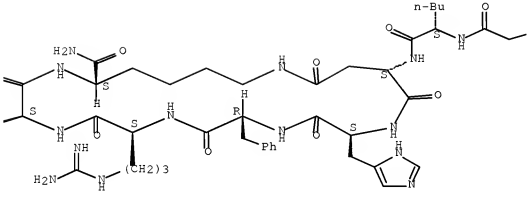
CN L-Lysinamide, N-[4-[(2-aminoethyl)[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]-1-oxobutyl]-β-alanyl-L-norleucyl-L-α-aspartyl-L-histidyl-D-phenylalanyl-L-arginyl-L-tryptophyl-, (3→8)-lactam (CA INDEX NAME)

Absolute stereochemistry.

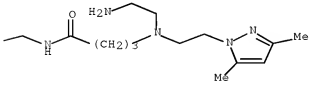
PAGE 1-A



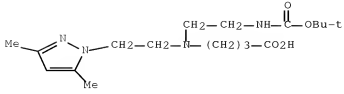
PAGE 1-B



PAGE 1-C



IT 782501-78-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(comparisons of solid-phase synthetic approaches to tumor-seeking α-MSH analog)
RN 782501-78-4 HCAPLUS
CN Butanoic acid, 4-[[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl][2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]- (CA INDEX NAME)



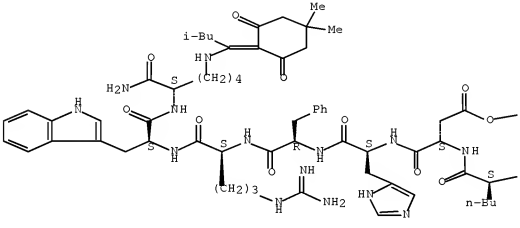
IT 1084652-81-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(comparisons of solid-phase synthetic approaches to tumor-seeking α-MSH analog)

RN 1084652-81-2 HCAPLUS

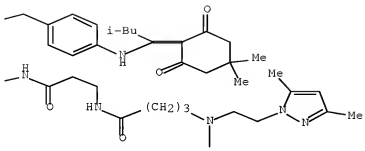
CN L-Lysinamide, N-[4-[[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl][2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]-1-oxobutyl]-β-alanyl-L-norleucyl-L-α-asparty l-L-histidyl-D-phenylalanyl-L-arginyl-L-tryptophyl-N6-[1-(4,4-dimethyl-2,6-dioxocyclohexylidene)-3-methylbutyl]-, [4-[[1-(4,4-dimethyl-2,6-dioxocyclohexylidene)-3-methylbutyl]amino]phenyl]methyl ester (CA INDEX NAME)

Absolute stereochemistry.

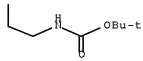
PAGE 1-A



PAGE 1-B



PAGE 2-B



REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 15 OF 21 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2007:605111 HCAPLUS Full-text
DOCUMENT NUMBER: 147:229603
TITLE: A new bisphosphonate-containing 99mTc(I) tricarbonyl complex potentially useful as bone-seeking agent: synthesis and biological evaluation
AUTHOR(S): Palma, Elisa; Oliveira, Bruno L.; Correia, Joao D. G.; Gano, Lurdes; Maria, Leonor; Santos, Isabel C.; Santos, Isabel
CORPORATE SOURCE: Departamento de Quimica, ITN, Sacavem Codex, 2686-953, Port.
SOURCE: JBIC, Journal of Biological Inorganic Chemistry (2007), 12(5), 667-679
CODEN: JJBCFA; ISSN: 0949-8257
PUBLISHER: Springer GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 05 Jun 2007
AB Aiming to develop new bone-seeking radiotracers based on the organometallic core fac-[99mTc(CO)3]+ with improved radiochem. and biol. properties, we have prepared new conjugates with phosphonate pendant groups. The conjugates comprise a chelating unit for metal coordination, which corresponds to a pyrazolyl-containing backbone (pz) with a N,N,N donor-atom set, and a pendant

di-Et phosphonate (pz-MPOEt), phosphonic acid (pz-MPOH) or a bisphosphonic acid (pz-BPOH) group for bone targeting. Reactions of the conjugates with the precursor [99mTc(H2O)3(CO)3]+ yielded (mote than 95%) the single and well-defined radioactive species [99mTc(CO)3(κ3-pz-MPOEt)]+ (1a), [99mTc(CO)3(κ3-pz-MPOH]+ (2a) and [99mTc(CO)3(κ3-pz-BPOH)]+ (3a), which were characterized by reversed-phase high-performance liquid chromatog. . The corresponding Re surrogates (1-3), characterized by the usual anal. techniques, including X-ray diffraction anal. in the case of 1, allowed for macroscopic identification of the radioactive conjugates. These radioactive complexes revealed high stability both in vitro (phosphate-buffered saline solution and human plasma) and in vivo, without any measurable decomposition Biodistribution studies of the complexes in mice indicated a fast rate of blood clearance and high rate of total radioactivity excretion, occurring primarily through the renal-urinary pathway in the case of complex 3a. Despite presenting moderate bone uptake (3.04 ± 0.47% injected dose per g of organ, 4 h after injection), the high stability presented by 3a and its adequate in vivo pharmacokinetics encourages the search for new ligands with the same chelating unit and different bisphosphonic acid pendant arms.

CC 8-9 (Radiation Biochemistry)

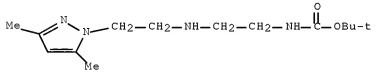
IT 5324-30-1 14220-21-4 25908-22-9 80474-99-3 782501-76-2
782501-78-4 850480-66-9 945384-86-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(bisphosphonate-containing 99mTc(I) tricarbonyl complex: preparation and potential as bone-seeking agent)

IT 945264-41-5P 945264-42-6P 945264-43-7P
945264-45-9P 945264-46-0P 945384-90-7P 945384-92-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(bisphosphonate-containing 99mTc(I) tricarbonyl complex: preparation and potential as bone-seeking agent)

IT 782501-76-2 782501-78-4 850480-66-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(bisphosphonate-containing 99mTc(I) tricarbonyl complex: preparation and potential as bone-seeking agent)

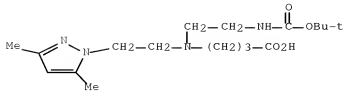
RN 782501-76-2 HCAPLUS

CN Carbamic acid, N-[2-[[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]ethyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

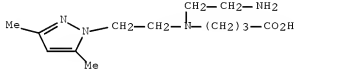


RN 782501-78-4 HCAPLUS

CN Butanoic acid, 4-[[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl][2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]- (CA INDEX NAME)

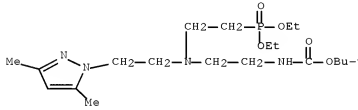


RN 850480-66-9 HCAPLUS
CN Butanoic acid, 4-[(2-aminoethyl)[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]- (CA INDEX NAME)

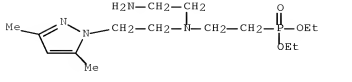


IT 945264-41-5P 945264-42-6P 945264-43-7P
945264-45-9P 945264-46-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(bisphosphonate-containing 99mTc(I) tricarbonyl complex: preparation and potential as bone-seeking agent)

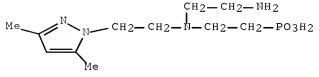
RN 945264-41-5 HCAPLUS
CN 9-Oxa-2,5-diaza-8-phosphaundecanoic acid, 5-[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]-8-ethoxy-, 1,1-dimethylethyl ester, 8-oxide (CA INDEX NAME)



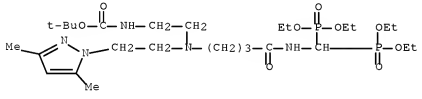
RN 945264-42-6 HCAPLUS
CN Phosphonic acid, P-[2-[(2-aminoethyl)[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]ethyl]-, diethyl ester (CA INDEX NAME)



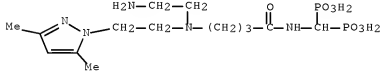
RN 945264-43-7 HCAPLUS
CN Phosphonic acid, P-[2-[(2-aminoethyl)[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]ethyl]- (CA INDEX NAME)



RN 945264-45-9 HCAPLUS
CN 13-Oxa-2,5,10-triaza-12-phosphapentadecanoic acid, 11-(diethoxyphosphinyl)-5-[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]-12-ethoxy-9-oxo-, 1,1-dimethylethyl ester, 12-oxide (CA INDEX NAME)



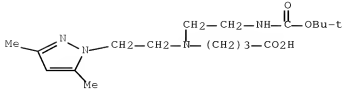
RN 945264-46-0 HCAPLUS
CN Phosphonic acid, P,P'-[[[4-[(2-aminoethyl)[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]-1-oxobutyl]amino]methylene]bis- (CA INDEX NAME)



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 16 OF 21 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2007:48914 HCAPLUS Full-text
DOCUMENT NUMBER: 146:311529
TITLE: In Vitro and In Vivo Evaluation of a Novel 99mTc(CO)3-Pyrazolyl Conjugate of cyclo-(Arg-Gly-Asp-D-Tyr-Lys)
AUTHOR(S): Alves, Susana; Correia, Joao D. G. ; Gano, Lurdes; Rold, Tammy L.; Prasanphanich, Adam; Haubner, Roland; Rupprich, Marco; Alberto, Roger;

Decristoforo, Clemens; Santos, Isabel; Smith, Charles J.
CORPORATE SOURCE: Department of Radiology Department of Internal Medicine and The Radiopharmaceutical Sciences Institute, University of Missouri-Columbia School of Medicine, Columbia, MO, 65211, USA
SOURCE: Bioconjugate Chemistry (2007), 18(2), 530-537 CODEN: BCCHES; ISSN: 1043-1802
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:311529
ED Entered STN: 16 Jan 2007
AB Radiolabeled peptides containing the Arg-Gly-Asp amino acid sequence (single letter code = RGD) have been studied extensively to target integrin receptors upregulated on tumor cells and neovasculature. Integrins are cell surface transmembrane glycoproteins that exist as αβ heterodimers. The αvβ3 integrin is known to be overexpressed in many tumor types and is expressed at lower levels in normal tissues. Furthermore, αvβ3 and αvβ5 subtypes are expressed in neovasculature during angiogenesis. Thus, there is some impetus to image angiogenesis and tumor formation in vivo using RGD-based peptide targeting vectors. In this study, we report the design and development of a new cyclic RGD analog cyclo-[Arg-Gly-Asp-D-Tyr-Lys(PZ)] (PZ = 3,5-Me2-pz(CH2)2N((CH2)3COOH)(CH2)2NH2) that can be radiolabeled with the [99mTc(CO)3(H2O)3]+ metal aquaion. Radiochem. evaluation of this new conjugate in vitro indicated a facile radiosynthesis of the new 99mTc-RGD conjugate with high radiolabeling yields (≥95%) and high specific activities. In vitro internalization and blocking assays in αvβ3 receptor-pos., human M21 melanoma cancer cells showed the ability of this conjugate to target the integrin receptor with high specificity and selectivity. In vivo pharmacokinetic studies in normal CF-1 mice showed rapid clearance from blood with excretion primarily via/through the renal-urinary system. In vivo accumulation of radioactivity in mice bearing either αvβ3 receptor-pos. or neg. human melanoma tumors showed receptor specific uptake of tracer with accumulations of 2.50 ± 0.29 and 0.71 ± 0.08% ID/g in αvβ3 integrin pos. (M21) and neg. (M21L) tumors at 1 h postinjection (p.i.), resp.
CC 8-9 (Radiation Biochemistry)
IT 163932-31-8 217099-14-4 782501-78-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(99mTc(CO)3-pyrazolyl conjugate of cyclo-(Arg-Gly-Asp-D-Tyr-Lys) preparation
and targeting integrin receptors in melanoma)
IT 928406-90-0P 928406-91-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(99mTc(CO)3-pyrazolyl conjugate of cyclo-(Arg-Gly-Asp-D-Tyr-Lys) preparation
and targeting integrin receptors in melanoma)
IT 782501-78-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(99mTc(CO)3-pyrazolyl conjugate of cyclo-(Arg-Gly-Asp-D-Tyr-Lys) preparation
and targeting integrin receptors in melanoma)
RN 782501-78-4 HCAPLUS
CN Butanoic acid, 4-[[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl][2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]- (CA INDEX NAME)



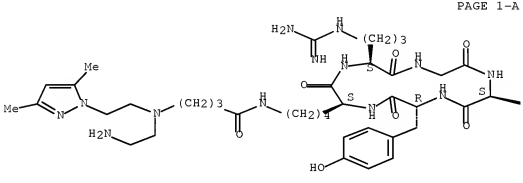
IT 928406-90-0P 928406-91-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(99mTc(CO)3-pyrazolyl conjugate of cyclo-(Arg-Gly-Asp-D-Tyr-Lys) preparation
and targeting integrin receptors in melanoma)

RN 928406-90-0 HCAPLUS

CN Cyclo[L-arginylglycyl-L-α-aspartyl-D-tyrosyl-N6-[4-[(2-aminoethyl)[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]-1-oxobutyl]-L-lysyl] (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



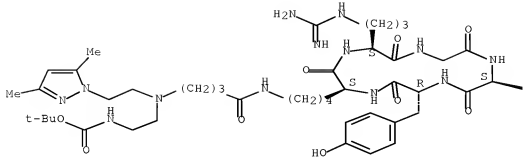
PAGE 1-B

RN 928406-91-1 HCAPLUS

CN Cyclo[L-arginylglycyl-L-α-aspartyl-D-tyrosyl-N6-[4-[[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl][2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]-1-oxobutyl]-L-lysyl] (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 17 OF 21 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2006:957931 HCAPLUS Full-text
DOCUMENT NUMBER: 147:202224
TITLE: Metal-based drugs for diagnosis and therapy
AUTHOR(S): Alves, Susana; Vitor, Rute; Raposinho, Paula D.; Marques, Fernanda; Correia, Joao D. G.; Paulo, Antonio; Santos, Isabel
CORPORATE SOURCE: Departamento de Quimica, Instituto Tecnologico e Nuclear, Sacavem, 2686-953, Port.
SOURCE: Metal Ions in Biology and Medicine (2006), 9, 3-8
CODEN: MIBMCT; ISSN: 1257-2535
PUBLISHER: John Libbey Eurotext
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 147:202224
ED Entered STN: 18 Sep 2006
AB The compound 3,5Me-pz(CH2)2NH(CH2)2NH2 (L1) is a very effective chelator for the fac-[M(CO)3(H2O)3]+ (M = Re (1) 99mTc (1a)) moieties, yielding the building blocks fac-[M(CO)3(k3-L1)]+ (M = Re (2) 99mTc (2a)). The evaluation of the in vitro and in vivo behavior of 2a showed that this stable building block displays a favorable biol. profile for labeling biomols. with 99mTc, biol. active peptides. Due to its versatility, L1 was integrated through its secondary amine into a peptide with affinity for MC1 receptors (L2), and derivatized with an anthracenyl group at the C(4) position of the pyrazolyl ring (L3). The resulting bifunctional chelators react with 1a yielding the

well defined fac-[99mTc(CO)3(k3-L)]+ (L = L2 (3a), L3 (4a)) complexes with excellent stability in vitro and in vivo. Complex 3a presents a significant internalization in B16F1 melanoma cells, showing in vivo a significant overall excretion and a reasonable tumor uptake, with a fast clearance from most organs and tissues. For complex 4a, in vitro studies using B16F1 melanoma cells showed significant nuclear internalization and an enhanced radiotoxicity for this compound, most probably due to the presence of the anthracenyl group which is a known DNA intercalator. The results obtained for complexes 3a and 4a indicate that this family of compds. is potentially useful to develop novel specific 99mTc radiopharmaceuticals directed for both detection and therapy of melanoma.

CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 1

ST rhenium aminoethylaminoethylpyrazole complex prepn; technetium aminoethylaminoethylpyrazole complex prepn; anthracenylmethyl deriv aminoethylaminoethylpyrazole rhenium technetium complex prepn antitumor activity; peptide sequence pyrazolyl chelator technetium complex prepn antitumor activity

IT Radiopharmaceuticals
(preparation of technetium-99m complexes with peptide sequence pyrazolyl chelator and (((aminoethyl)amino)ethyl)pyrazole anthracenylmethyl derivative for development of)

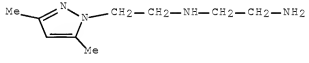
IT 511513-23-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of rhenium and technetium-99m complexes with (((aminoethyl)amino)ethyl)pyrazole and its derivs. with anthracenylmethyl and peptide sequence)

IT 944389-68-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with technetium-99m aqua carbonyl complex)

IT 511513-23-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of rhenium and technetium-99m complexes with (((aminoethyl)amino)ethyl)pyrazole and its derivs. with anthracenylmethyl and peptide sequence)

RN 511513-23-8 HCAPLUS

CN 1,2-Ethanediamine, N1-[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]- (CA INDEX NAME)



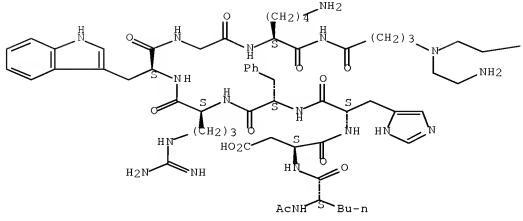
IT 944389-68-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with technetium-99m aqua carbonyl complex)

RN 944389-68-8 HCAPLUS

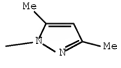
CN L-Lysinamide, N-acetyl-L-norleucyl-L-α-aspartyl-L-histidyl-L-phenylalanyl-L-arginyl-L-tryptophylglycyl-N-[4-[(2-aminoethyl)[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]amino]-1-oxobutyl]- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 18 OF 21 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2002:937047 HCAPLUS Full-text
DOCUMENT NUMBER: 138:330675
TITLE: Coordination capabilities of pyrazolyl containing ligands towards the fac-[Re(CO)3]+ moiety
AUTHOR(S): Alves, Susana; Paulo, Antonio; Correia, Joao D. G.; Domingos, Angela; Santos, Isabel
CORPORATE SOURCE: Departamento de Quimica, ITN, Sacavem, 2686-953, Port.
SOURCE: Journal of the Chemical Society, Dalton Transactions (2002), (24), 4714-4719
CODEN: JCSDAA; ISSN: 1472-7773
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:330675
ED Entered STN: 10 Dec 2002
AB The coordination capabilities of the pyrazolyl containing ligands pz*(CH2)2NH(CH2)2pz*, pz*(CH2)2NH(CH2)2NH2, pz*(CH2)2S(CH2)2pz* and pz*(CH2)2S(CH2)2NH2 (pz* = 3,5-Me2pz) towards the synthon (NEt4)2[ReBr3(CO)3] (1) were studied. Depending on the reaction conditions, neutral or cationic Re(I) tricarbonyl complexes were isolated: [ReBr(CO)3(κ2-pz*(CH2)2NH(CH2)2pz*)] (2), [ReBr(CO)3(κ2-pz*(CH2)2S(CH2)2pz*)] (3)

[Re(CO)3(κ3-pz*(CH2)2NH(CH2)2pz*)]Br (4), [Re(CO)3(κ2-pz*(CH2)2S(CH2)2pz*)MeOH]Br (5), [Re(CO)3(κ3-pz*(CH2)2NH(CH2)2NH2)]Br (6) and [Re(CO)3(κ3-pz*(CH2)2S(CH2)2NH2)]Br (7). Complexes 2-7 were characterized by the normal techniques, including x-ray crystallog. anal. in the case of 3, 4, 6 and 7. In these complexes the Re atom adopts a distorted octahedral coordination, being one of the triangular faces defined by the three carbonyl groups and the other three remaining coordination positions by the bidentate and the bromide ligands (3), or by the tridentate and neutral pyrazolyl containing ligands (4, 6, 7). Complexes 2-4, 6 and 7 are static in solution and the 1H NMR data indicate clearly a κ2-coordination mode of the ligand in 2 and 3 and a κ3-coordination in 4, 6 and 7, which agrees with the coordination mode found in the solid state. Compound 5 displays a fluxional behavior in solution as shown by variable temperature 1H NMR studies. No x-ray data exists for this complex but the pattern obtained for the NMR spectrum at 215 K indicates a κ2-coordination mode for the pyrazolyl containing ligand.

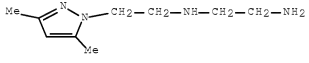
CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 75

IT 511513-23-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and complexation with rhenium carbonyl complex)

IT 511513-23-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and complexation with rhenium carbonyl complex)

RN 511513-23-8 HCAPLUS

CN 1,2-Ethanediamine, N1-[2-(3,5-dimethyl-1H-pyrazol-1-yl)ethyl]- (CA INDEX NAME)



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib ed ab ind 19-21
YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS, EMBASE, SCISEARCH' - CONTINUE? (Y)/N:y

L49 ANSWER 19 OF 21 EMBASE COPYRIGHT (c) 2009 Elsevier B.V. All rights reserved on STN

ACCESSION NUMBER: 2006052409 EMBASE Full-text
TITLE: Radiopharmaceuticals for targeted radiotherapy.
AUTHOR: Marques, Fernanda (correspondence); Paulo, Antonio ; Campello, Maria Paula; Lacerda, Sara; Vitor, Rute Filipe; Gano, Lurdes; Santos, Isabel
CORPORATE SOURCE: Departamento de Quimica, Instituto Tecnologico e Nuclear, EN 10, Apartado 21, 2686-953 Sacavem, Portugal. fmarujo@itn.mces.pt
AUTHOR: Delgado, Rita

CORPORATE SOURCE: Instituto Tecnologia Quimica e Biologica, UNL, Apartado 127, 2781-901 Oeiras, Portugal.
SOURCE: Radiation Protection Dosimetry, (20 Dec 2005) Vol. 116, No. 1-4, pp. 601-604.
Refs: 13
ISSN: 0144-8420 CODEN: RPDODE
COUNTRY: United Kingdom
DOCUMENT TYPE: Journal; Article
FILE SEGMENT: 016 Cancer
023 Nuclear Medicine
030 Clinical and Experimental Pharmacology
037 Drug Literature Index
039 Pharmacy
LANGUAGE: English
SUMMARY LANGUAGE: English
ENTRY DATE: Entered STN: 3 Mar 2006
Last Updated on STN: 3 Mar 2006

ED Entered STN: 3 Mar 2006
Last Updated on STN: 3 Mar 2006

AB This work intends to find specific radiopharmaceuticals for cancer therapy based on beta ((153)Sm and (166)Ho) or Auger ((99)Tc(m)) emitter radionuclides, using cyclic and acyclic polyamines as bifunctional chelators. These chelators are designed to allow the binding of a tumour seeking biomolecule and/or a DNA intercalator. The cyclic amines, such as 1,4,7,10-tetraazacyclododecane-1,4,7,10-tetraacetic acid, 1,4,8,11-tetraazacyclotetradecane-1,4,8,11-tetraacetic acid and 1,4,7,10-tetraazacyclotridecane-1,4,7,10-tetraacetic acid, were radiolabelled with (153)Sm and (166)Ho. The radiochemical and biological behaviour of the resulting complexes were evaluated in order to assess their potential as building blocks for the attachment of selected biomolecules, with the aim of further applying them for the development of specific therapeutic radiopharmaceuticals. Novel pyrazolyldiamines, bearing a DNA intercalating anthracenyl fragment, were also explored to synthesize radioactive complexes with the fac- (99)Tc(m)(CO) (3) (+) moiety. The identity of these (99)Tc(m) tricarbonyl complexes was confirmed by high-performance liquid chromatography comparison with rhenium congeners fully characterized. By including a DNA intercalator into the chelator framework, we expect to induce more efficient and selective damage to the DNA of cancer cells by the action of the short-range Auger electrons emitted by (99)Tc(m). .COPYRGT. The Author 2005. Published by Oxford University Press. All rights reserved.

CT Medical Descriptors:
article
beta radiation
cancer cell
*cancer radiotherapy
clinical trial
complex formation
DNA damage
drug binding
drug determination
drug selectivity
drug structure
drug synthesis
drug targeting
human
isotope labeling
radiochemistry
reversed phase high performance liquid chromatography

CT Drug Descriptors:
1,4,7,10 tetraazacyclododecane 1,4,7,10 tetraacetic acid

1,4,7,10 tetraazacyclotridecane 1,4,7,10 tetraacetic acid
1,4,8,11 tetraazacyclotetradecane 1,4,8,11 tetraacetic acid
anthracene derivative
chelating agent
cyclam derivative
holmium: PR, pharmaceutics
holmium: PD, pharmacology
holmium 166: PR, pharmaceutics
holmium 166: PD, pharmacology
intercalating agent
losoxantrone: CT, clinical trial
losoxantrone: AN, drug analysis
losoxantrone: PR, pharmaceutics
losoxantrone: PD, pharmacology
polyamine derivative
pyrazolyldiamine derivative: PR, pharmaceutics
pyrazolyldiamine derivative: PD, pharmacology
radioisotope: PR, pharmaceutics
radioisotope: PD, pharmacology
*radiopharmaceutical agent: CT, clinical trial
*radiopharmaceutical agent: AN, drug analysis
*radiopharmaceutical agent: PR, pharmaceutics
*radiopharmaceutical agent: PD, pharmacology
rhenium complex
samarium 153: PR, pharmaceutics
samarium 153: PD, pharmacology
technetium 99m: PR, pharmaceutics
technetium 99m: PD, pharmacology
unclassified drug

RN (1,4,7,10 tetraazacyclododecane 1,4,7,10 tetraacetic acid) 60239-18-1; (holmium) 7440-60-0; (losoxantrone) 88303-60-0; (samarium 153) 15766-00-4; (technetium 99m) 14133-76-7

L49 ANSWER 20 OF 21 SCISEARCH COPYRIGHT (c) 2009 The Thomson Corporation on STN

ACCESSION NUMBER: 2009:366412 SCISEARCH Full-text
THE GENUINE ARTICLE: 417GQ
TITLE: Influence of the ligand donor atoms on the in vitro stability of rhenium(I) and technetium (I)-99m complexes with pyrazole-containing chelators: Experimental and DFT studies
AUTHOR: Santos, Isabel (Reprint)
CORPORATE SOURCE: ITN, Unidade Ciencias Quim & Radiofarmaceut, Estr Nacl 10, P-2686953 Sacavem Codex, Portugal (Reprint)
E-mail: isantos@itn.pt
AUTHOR: Santos, Isabel (Reprint)
CORPORATE SOURCE: ITN, Unidade Ciencias Quim & Radiofarmaceut, P-2686953 Sacavem Codex, Portugal
E-mail: isantos@itn.pt
AUTHOR: Moura, Carolina; Fernandes, Celia; Gano, Lurdes; Paulo, Antonio; Santos, Isabel C.; Calhorda, Maria Jose
CORPORATE SOURCE: Univ Lisbon, Dept Quim & Bioquim, CQB, Fac Ciencias, P-1749016 Lisbon, Portugal
COUNTRY OF AUTHOR: Portugal
SOURCE: JOURNAL OF ORGANOMETALLIC CHEMISTRY, (15 MAR 2009) Vol. 694, No. 6, pp. 950-958.
ISSN: 0022-328X.
PUBLISHER: ELSEVIER SCIENCE SA, PO BOX 564, 1001 LAUSANNE, SWITZERLAND.

DOCUMENT TYPE: Article; Journal
LANGUAGE: English
REFERENCE COUNT: 63
ENTRY DATE: Entered STN: 26 Mar 2009
Last Updated on STN: 7 May 2009
ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

ED Entered STN: 26 Mar 2009
Last Updated on STN: 7 May 2009

AB The new pyrazole-containing ligand 3,5-Me(2)pz(CH2)(2)S(CH2)(2)COOH ((LH)-H-1)was synthesized and used to prepare the complexes fac-[M(kappa(3)-L-1)(CO)(3)] (M = Re (1), (99mt)c(1a)), which were obtained in high yield albeit with a low specific activity in the case of Tc-99m. The X-ray diffraction analysis of 1 confirmed that L-1 coordinates to the metal as monoanionic and through a (N,S,O) donor atom set. Challenge experiments of 1a against cysteine and histidine showed that this complex suffers considerable transchelation in vitro. This contrasts with the behavior exhibited by the related complex fac-[Tc-99m(kappa(3)-L-2)(CO)(3)](2a)(L-2 = 3,5-Me(2)pz-(CH2)(2)NH-CH2-COO), anchored by a (N2O)-tridentate ligand. Biodistribution studies of 1a and 2a in mice indicated that both compounds have a relatively similar biological profile. Nevertheless, the fastest blood clearance and minor hepatic retention found for 2a has shown that this complex is more adequate to be further explored in radiopharmaceutical sciences. DFT calculations (ADF program)were performed for these neutral complexes and related cationic M(I)(M = Re, Tc) tricarbonyl complexes anchored by pyrazole-containing ligands, in order to have a better understanding of the influence of the donor atom set (N,N,O vs. N,O,S; N,N,N vs. N,N,S vs. N,S,S)on their in vitro stability. The differences of the calculated binding energies are not significant, suggesting that the in vitro behavior of these Re(I)/Tc(I)tricarbonyl complexes is not determined by thermodynamic factors. (C) 2008 Elsevier B. V. All rights reserved.

CC CHEMISTRY, INORGANIC & NUCLEAR; CHEMISTRY, ORGANIC

ST Author Keywords: Rhenium; Technetium; Carbonyl; Pyrazolyl -containing ligands; DFT calculations

STP KeyWords Plus (R): TRANSITION-STATE METHOD; REGULAR 2-COMPONENT HAMILTONIANS; DENSITY-FUNCTIONAL THEORY; TRICARBONYL COMPLEXES; SCREENING MODEL; VIVO EVALUATION; RADIOPHARMACEUTICALS; APPROXIMATION; BIOMOLECULES; DERIVATIVES
ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

L49 ANSWER 21 OF 21 SCISEARCH COPYRIGHT (c) 2009 The Thomson Corporation on STN

ACCESSION NUMBER: 1999:482083 SCISEARCH Full-text
THE GENUINE ARTICLE: 209HU
TITLE: Derivative chemistry of [UCl2{B(pz)(4)}(2)]: stability of complexes containing the fragments [U{B(pz)(4)}(2)] and [U{HB(pz)(3)}(2)]
AUTHOR: Santos I (Reprint)
CORPORATE SOURCE: ITN, Dept Quim, P-2686 Sacavem, Portugal (Reprint)
AUTHOR: Campello M P C; Domingos A; Galvao A; de Matos A P
CORPORATE SOURCE: Inst Super Tecn, Dept Engn Quim, P-1096 Lisbon, Portugal
COUNTRY OF AUTHOR: Portugal
SOURCE: JOURNAL OF ORGANOMETALLIC CHEMISTRY, (5 MAY 1999) Vol. 579, No. 1-2, pp. 5-17.
ISSN: 0022-328X.
PUBLISHER: ELSEVIER SCIENCE SA, PO BOX 564, 1001 LAUSANNE, SWITZERLAND.
DOCUMENT TYPE: Article; Journal
LANGUAGE: English
REFERENCE COUNT: 42

ENTRY DATE: Entered STN: 1999
Last Updated on STN: 1999
ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

ED Entered STN: 1999
Last Updated on STN: 1999

AB Uranium tetrachloride reacts with two equivalents of K[B(pz)(4)] in THF affording [UCl2{B(pz)(4)}(2)] (1) in 75% yield. Complex 1 is monomeric and crystallizes in the monoclinic space group C2/c with cell parameters a = 13.700(6), b = 12.759(2), c = 17.513(8) Angstrom, beta = 101.37(2)degrees, V = 3001(2) Angstrom(3), Z = 4. Derivatives [UCl(OR){B(pz)(4)}(2)] (R=C2H5 (2), Bu-t (3), C6H4-o-OMe (4) and C6H2-2,4,6-Me-3 (5)), [U((OBu)-Bu-t)(2){B(pz)(4)}(2)] (6), [U((SPr)-Pr-i)(2){B(pz)(4)}(2)] (7) and [UCl(Me){B(pz)(4)}(2)] (8) were obtained by reacting 1 with sodium alkoxides, with (NaSPr)-Pr-i or with LiMe. X-ray crystallographic analysis of 5 and 7 shows that uranium is eight-coordinate by the two eta(3)-[B(pz)(4)] ligands and by two monodentate coligands (5. crystallizes in the monoclinic space group C2/c with cell parameters a = 30.575(3). b = 9.929(1), c = 24.884(3) Angstrom, beta = 90.59(1)degrees, V = 7554(1) Angstrom(3), Z = 8; 7 crystallizes in the monoclinic space group C2/c with cell parameters a = 24.286(7), b = 9.471(2), c = 16.076(3) Angstrom, beta = 96.44(3)degrees, V = 3674(2) Angstrom(3), Z = 4). Extended Huckel molecular orbital (EHMO) calculations were used to get a better insight into the electronic properties of the ligand [B(pz)(4)] and to get some explanation on the relative stability of complexes containing the fragments '[U(B(pz)(4)}(2)] and '[U(HB(pz)(3)}(2)]'. (C) 1999 Elsevier Science S.A. All rights reserved.

CC CHEMISTRY, INORGANIC & NUCLEAR; CHEMISTRY, ORGANIC

ST Author Keywords: uranium; poly(pyrazolyl)borates; EHMO calculations; stability

STP KeyWords Plus (R): ION SIZE DISCRIMINATION; X-RAY CRYSTAL; POLY(PYRAZOLYL)BORATE LIGANDS; MOLECULAR-STRUCTURES; CHELATE COMPLEXES; LANTHANIDE IONS; INTRALIGAND; CONTACT; MODE
ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

=> file stnguide
FILE 'STNGUIDE' ENTERED AT 13:45:22 ON 25 JUN 2009
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Jun 19, 2009 (20090619/UP).

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=> d his ful

     (FILE 'HOME' ENTERED AT 12:43:21 ON 25 JUN 2009)

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     FILE 'ZCAPLUS' ENTERED AT 12:44:29 ON 25 JUN 2009
                E US2005-551292/APPS

     FILE 'HCAPLUS' ENTERED AT 12:44:45 ON 25 JUN 2009
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                  D SCAN

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     FILE 'WPIX' ENTERED AT 12:45:26 ON 25 JUN 2009
L2             1 SEA SPE=ON  ABB=ON  PLU=ON  US2005-551292/APPS
                  D IALL CODE

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     FILE 'REGISTRY' ENTERED AT 12:47:09 ON 25 JUN 2009

     FILE 'HCAPLUS' ENTERED AT 12:47:12 ON 25 JUN 2009
L3               TRA PLU=ON  L1 1- RN :       29 TERMS

     FILE 'REGISTRY' ENTERED AT 12:47:14 ON 25 JUN 2009
L4            29 SEA SPE=ON  ABB=ON  PLU=ON  L3
                  D SCAN

     FILE 'STNGUIDE' ENTERED AT 12:47:38 ON 25 JUN 2009

     FILE 'LREGISTRY' ENTERED AT 12:49:19 ON 25 JUN 2009
L5               STR

     FILE 'REGISTRY' ENTERED AT 12:54:28 ON 25 JUN 2009
L6             5 SEA SSS SAM L5

     FILE 'STNGUIDE' ENTERED AT 12:54:53 ON 25 JUN 2009
                  D QUE STAT

     FILE 'REGISTRY' ENTERED AT 12:59:40 ON 25 JUN 2009
L7           827 SEA SSS FUL L5
                  SAVE TEMP L7 SCH292PSET1/A
L8            10 SEA SPE=ON  ABB=ON  PLU=ON  L4 AND L7
L9            19 SEA SPE=ON  ABB=ON  PLU=ON  L4 NOT L8
                  D SCAN

     FILE 'STNGUIDE' ENTERED AT 13:01:33 ON 25 JUN 2009

     FILE 'LREGISTRY' ENTERED AT 13:02:03 ON 25 JUN 2009
L10              STR L5

     FILE 'REGISTRY' ENTERED AT 13:03:00 ON 25 JUN 2009
L11            2 SEA SUB=L7 SSS SAM L10
                  D SCAN
L12           90 SEA SUB=L7 SSS FUL L10
                  SAVE TEMP L12 SCH292RSET1/A
L13            0 SEA SPE=ON  ABB=ON  PLU=ON  L8 NOT L12
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     FILE 'STNGUIDE' ENTERED AT 13:05:03 ON 25 JUN 2009

     FILE 'REGISTRY' ENTERED AT 13:06:34 ON 25 JUN 2009

     FILE 'ZCAPLUS' ENTERED AT 13:07:06 ON 25 JUN 2009
L*** DEL        QUE SANTOS, I?/AU
L*** DEL        QUE REGO, I?/AU
L14             QUE SPE=ON  ABB=ON  PLU=ON  SANTOS, I?/AU,AUTH
L15             QUE SPE=ON  ABB=ON  PLU=ON  REGO, I?/AU,AUTH
L16             QUE SPE=ON  ABB=ON  PLU=ON  CORREIA, J?/AU,AUTH
L17             QUE SPE=ON  ABB=ON  PLU=ON  PAULO, A?/AU,AUTH
L18             QUE SPE=ON  ABB=ON  PLU=ON  ALVES, S?/AU,AUTH
L19             QUE SPE=ON  ABB=ON  PLU=ON  VITOR, R?/AU,AUTH
L20             QUE SPE=ON  ABB=ON  PLU=ON  MALLINCKRODT/CS,SO,PA
L21             QUE SPE=ON  ABB=ON  PLU=ON  AY<2004 OR PY<2004 OR PRY<2004 OR
                MY<2004 OR REVIEW/DT
L22             QUE SPE=ON  ABB=ON  PLU=ON  BIOMOLECUL? OR (BIO(1W)MOLECUL?)
                OR (BIOLOGIC?(3A)MOLECUL?)
L23             QUE SPE=ON  ABB=ON  PLU=ON  CHELAT?
L24             QUE SPE=ON  ABB=ON  PLU=ON  "CHELATING AGENTS"+PFT,OLD,NEW,NT/C
                T

     FILE 'HCAPLUS' ENTERED AT 13:21:41 ON 25 JUN 2009
L25         46 SEA SPE=ON  ABB=ON  PLU=ON  L12
L26         19 SEA SPE=ON  ABB=ON  PLU=ON  L25 AND (L22 OR L23 OR L24)
L27         46 SEA SPE=ON  ABB=ON  PLU=ON  (L25 OR L26)
L28         18 SEA SPE=ON  ABB=ON  PLU=ON  L27 AND (L14 OR L15 OR L16 OR L17
                OR L18 OR L19 OR L20)
L29         28 SEA SPE=ON  ABB=ON  PLU=ON  L27 NOT L28
L30         23 SEA SPE=ON  ABB=ON  PLU=ON  L29 AND L21
L31         28 SEA SPE=ON  ABB=ON  PLU=ON  (L29 OR L30)

     FILE 'WPIX' ENTERED AT 13:24:10 ON 25 JUN 2009
                D QUE L12
L32          2 SEA SSS SAM L10
                D TRI 1-2
L33         10 SEA SSS FUL L10
                SAVE TEMP L33 SCH292WPIS/A
                SELECT L33 1- SDCN
L34          3 SEA SPE=ON  ABB=ON  PLU=ON  (RABNX7/DCN OR RAFVJB/DCN OR
                RAFVJC/DCN OR RAFVJD/DCN OR RAFVJE/DCN OR RAFVJF/DCN OR
                RAFVJG/DCN OR RAFVJ8/DCN OR RAFVJ9/DCN OR RAMT8E/DCN) OR
                L33/DCR
L35          2 SEA SPE=ON  ABB=ON  PLU=ON  L34 AND (L22 OR L23)
L36          3 SEA SPE=ON  ABB=ON  PLU=ON  (L34 OR L35)
L37          1 SEA SPE=ON  ABB=ON  PLU=ON  L36 AND (L14 OR L15 OR L16 OR L17
                OR L18 OR L19 OR L20)
L38          2 SEA SPE=ON  ABB=ON  PLU=ON  L36 NOT L37
                D TRI HITSTR 1-2

     FILE 'STNGUIDE' ENTERED AT 13:27:39 ON 25 JUN 2009

     FILE 'MEDLINE' ENTERED AT 13:28:54 ON 25 JUN 2009
L39          0 SEA SPE=ON  ABB=ON  PLU=ON  L12

     FILE 'REGISTRY' ENTERED AT 13:29:10 ON 25 JUN 2009
L40         10 SEA SPE=ON  ABB=ON  PLU=ON  L4 AND L12

     FILE 'MEDLINE' ENTERED AT 13:29:34 ON 25 JUN 2009
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                SET SMARTSELECT OFF

     FILE 'MEDLINE' ENTERED AT 13:29:40 ON 25 JUN 2009

     FILE 'EMBASE' ENTERED AT 13:29:56 ON 25 JUN 2009
L41             0 SEA SPE=ON  ABB=ON  PLU=ON  L12

     FILE 'STNGUIDE' ENTERED AT 13:30:05 ON 25 JUN 2009

     FILE 'BIOSIS, CABA, AGRICOLA, BIOTECHNO, DRUGU, VETU' ENTERED AT 13:30:22
     ON 25 JUN 2009
L42             0 SEA SPE=ON  ABB=ON  PLU=ON  L12

     FILE 'STNGUIDE' ENTERED AT 13:30:39 ON 25 JUN 2009

     FILE 'MEDLINE, BIOSIS, EMBASE, PASCAL, JAPIO, CABA, CEABA-VTB, LIFESCI,
     BIOENG, BIOTECHNO, BIOTECHDS, DRUGU, DRUGB, VETU, VETB, SCISEARCH,
     CONFSCI, DISSABS, RDISCLOSURE' ENTERED AT 13:31:47 ON 25 JUN 2009
L43           769 SEA SPE=ON  ABB=ON  PLU=ON  ?PYRAZOL?/IT,TI,CC,CT,ST,STP AND
                  L23/IT,TI,CC,CT,ST,STP
L44            20 SEA SPE=ON  ABB=ON  PLU=ON  L43 AND (L14 OR L15 OR L16 OR L17
                  OR L18 OR L19 OR L20)

     FILE 'STNGUIDE' ENTERED AT 13:33:10 ON 25 JUN 2009
                D QUE STAT L7
                D QUE STAT L12
                D QUE NOS L31
                D QUE STAT L33
                D QUE NOS L38
                D QUE NOS L39
                D QUE NOS L41
                D QUE NOS L42

     FILE 'HCAPLUS, WPIX' ENTERED AT 13:37:35 ON 25 JUN 2009
L45            28 DUP REM L31 L38 L39 L41 L42 (2 DUPLICATES REMOVED)
                       ANSWERS '1-27' FROM FILE HCAPLUS
                       ANSWER '28' FROM FILE WPIX
                SAVE TEMP L45 SCH292MAINP/A

     FILE 'STNGUIDE' ENTERED AT 13:37:48 ON 25 JUN 2009

     FILE 'HCAPLUS, WPIX' ENTERED AT 13:38:10 ON 25 JUN 2009
                D QUE L21
L*** DEL       28 S L29-L30
L*** DEL        2 S L36 NOT L37
L46            23 SEA SPE=ON  ABB=ON  PLU=ON  L45 AND L21
L47            23 DUP REM L46 (0 DUPLICATES REMOVED)
                       ANSWERS '1-22' FROM FILE HCAPLUS
                       ANSWER '23' FROM FILE WPIX

     FILE 'STNGUIDE' ENTERED AT 13:39:14 ON 25 JUN 2009

     FILE 'HCAPLUS, WPIX' ENTERED AT 13:39:20 ON 25 JUN 2009
                D IBIB ED ABS HITIND HITSTR 1-22

     FILE 'STNGUIDE' ENTERED AT 13:39:37 ON 25 JUN 2009
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     FILE 'HCAPLUS, WPIX' ENTERED AT 13:41:17 ON 25 JUN 2009
                D IALL ABEQ TECH ABEX FRAGHITSTR 23

     FILE 'STNGUIDE' ENTERED AT 13:41:18 ON 25 JUN 2009

     FILE 'HCAPLUS, WPIX' ENTERED AT 13:41:34 ON 25 JUN 2009
L*** DEL     28 S L29-L30
L*** DEL     22 S L45 AND L21
L*** DEL      2 S L36 NOT L37
L*** DEL      1 S L45 AND L21
L48           5 SEA SPE=ON  ABB=ON  PLU=ON  L45 NOT L47

     FILE 'STNGUIDE' ENTERED AT 13:41:51 ON 25 JUN 2009

     FILE 'HCAPLUS' ENTERED AT 13:41:55 ON 25 JUN 2009
                D IBIB ED ABS HITIND HITSTR 1-5

     FILE 'STNGUIDE' ENTERED AT 13:42:02 ON 25 JUN 2009
                D QUE NOS L28
                D QUE NOS L37
                D QUE NOS L39
                D QUE NOS L41
                D QUE NOS L42
                D QUE L44

     FILE 'HCAPLUS, WPIX, MEDLINE, BIOSIS, EMBASE, PASCAL, BIOENG, SCISEARCH'
     ENTERED AT 13:43:20 ON 25 JUN 2009
L49           21 DUP REM L28 L37 L39 L41 L42 L44 (18 DUPLICATES REMOVED)
                     ANSWERS '1-18' FROM FILE HCAPLUS
                     ANSWER '19' FROM FILE EMBASE
                     ANSWERS '20-21' FROM FILE SCISEARCH
                SAVE TEMP L49 SCH292INV/A

     FILE 'STNGUIDE' ENTERED AT 13:43:36 ON 25 JUN 2009

     FILE 'HCAPLUS, EMBASE, SCISEARCH' ENTERED AT 13:43:55 ON 25 JUN 2009
                D IBIB ED ABS HITIND HITSTR 1-18

     FILE 'STNGUIDE' ENTERED AT 13:44:05 ON 25 JUN 2009

     FILE 'HCAPLUS, EMBASE, SCISEARCH' ENTERED AT 13:45:06 ON 25 JUN 2009
                D IBIB ED AB IND 19-21

     FILE 'STNGUIDE' ENTERED AT 13:45:07 ON 25 JUN 2009

     FILE 'STNGUIDE' ENTERED AT 13:45:22 ON 25 JUN 2009


     FILE HOME

     FILE STNGUIDE
     FILE CONTAINS CURRENT INFORMATION.
     LAST RELOADED: Jun 19, 2009 (20090619/UP).

     FILE ZCAPLUS

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FILE COVERS 1907 - 25 Jun 2009 VOL 150 ISS 26
FILE LAST UPDATED: 24 Jun 2009 (20090624/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Apr 2009

ZCAplus now includes complete International Patent Classification (IPC)
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FILE COVERS 1907 - 25 Jun 2009 VOL 150 ISS 26
FILE LAST UPDATED: 24 Jun 2009 (20090624/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2009
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FILE WPIX
FILE LAST UPDATED: 19 JUN 2009 <20090619/UP>
MOST RECENT UPDATE: 200939 <200939/DW>
DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE
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>>> IPC, ECLA and US National Classifications have been updated
with reclassifications to March 15th, 2009.
F-Term and FI-Term original classifications are current and
reclassification will commence in June.
No update date (UP) has been created for the reclassified
documents, but they can be identified by

specific update codes (see HELP CLA for details)<<<

FOR A COPY OF THE DERWENT WORLD PATENTS INDEX STN USER GUIDE,
PLEASE VISIT:
http://www.stn-international.com/stn_guide.html

FOR DETAILS OF THE PATENTS COVERED IN CURRENT UPDATES, SEE
http://scientific.thomsonreuters.com/support/patents/coverage/latestupdate

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>>> HELP for European Patent Classifications see HELP ECLA, HELP ICO <<<

FILE REGISTRY
Property values tagged with IC are from the ZIC/VINITI data file
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STRUCTURE FILE UPDATES: 23 JUN 2009 HIGHEST RN 1159631-40-9
DICTIONARY FILE UPDATES: 23 JUN 2009 HIGHEST RN 1159631-40-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

Please note that search-term pricing does apply when
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FILE LREGISTRY
LREGISTRY IS A STATIC LEARNING FILE

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FILE MEDLINE
FILE LAST UPDATED: 24 Jun 2009 (20090624/UP). FILE COVERS 1949 TO DATE.

MEDLINE and LMEDLINE have been updated with the 2009 Medical Subject
Headings (MeSH) vocabulary and tree numbers from the U.S. National Libra
of Medicine (NLM). Additional information is available at

http://www.nlm.nih.gov/pubs/techbull/nd08/nd08_medline_data_changes_2009.

On February 21, 2009, MEDLINE was reloaded. See HELP RLOAD for details.

This file contains CAS Registry Numbers for easy and accurate
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See HELP RANGE before carrying out any RANGE search.

FILE EMBASE
FILE COVERS 1974 TO 25 Jun 2009 (20090625/ED)

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 EMBASE was reloaded on March 30, 2008.

 EMBASE is now updated daily.  SDI frequency remains weekly (default)
 and biweekly.

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 substance identification.

 Beginning January 2008, Elsevier will no longer provide EMTREE
 codes as part of the EMTREE thesaurus in EMBASE.  Please update
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 For further assistance, please contact your local helpdesk.

FILE BIOSIS
FILE COVERS 1926 TO DATE.
CAS REGISTRY NUMBERS AND CHEMICAL NAMES (CNs) PRESENT
FROM JANUARY 1926 TO DATE.

RECORDS LAST ADDED: 24 June 2009 (20090624/ED)

BIOSIS has been augmented with 1.8 million archival records from 1926
through 1968.  These records have been re-indexed to match current
BIOSIS indexing.

FILE CABA
FILE COVERS 1973 TO 4 Jun 2009 (20090604/ED)

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The CABA file was reloaded 7 December 2003.  Enter HELP RLOAD for details.

FILE AGRICOLA

FILE COVERS 1970 TO 10 Jun 2009 (20090610/ED)

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FILE LAST UPDATED: 7 JAN 2004       <20040107/UP>
FILE COVERS 1980 TO 2003.
THIS FILE IS A STATIC FILE WITH NO UPDATES

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FILE DRUGU
FILE LAST UPDATED: 24 JUN 2009       <20090624/UP>
>>>  DERWENT DRUG FILE (SUBSCRIBER)  <<<

>>>  FILE COVERS 1983 TO DATE  <<<
>>>  THESAURUS AVAILABLE IN /CT  <<<
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FILE VETU
FILE LAST UPDATED: 2 JAN 2002       <20020102/UP>
FILE COVERS 1983-2001


FILE PASCAL
FILE LAST UPDATED: 22 JUN 2009       <20090622/UP>
FILE COVERS 1977 TO DATE.

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FILE JAPIO
FILE LAST UPDATED:            8 JUN 2009       <20090608/UP>
MOST RECENT PUBLICATION DATE: 26 FEB 2009       <20090226/PD>

>>> GRAPHIC IMAGES AVAILABLE <<<

FILE CEABA-VTB
FILE LAST UPDATED: 25 JUN 2009       <20090625/UP>
FILE COVERS 1966 TO DATE

>>> DECHEMA, the producer of CEABA-VTB is using a new classification
    scheme.
    The new classification schemes are available as a PDF file
    and may be downloaded free-of-charge from:
    http://www.stn-international.com/cc-de.html
    and
    http://www.stn-international.com/cc-en.html<<<

FILE LIFESCI
FILE COVERS 1978 TO 1 May 2009 (20090501/ED)

FILE BIOENG
FILE LAST UPDATED: 3 JUN 2009       <20090603/UP>
FILE COVERS 1982 TO DATE

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FILE BIOTECHDS
FILE LAST UPDATED: 19 JUN 2009       <20090619/UP>
FILE COVERS 1982 TO DATE

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FILE DRUGB
 >>>  FILE COVERS 1964 TO 1982 - CLOSED FILE  <<<


FILE VETB
FILE LAST UPDATED: 25 SEP 94      <940925/UP>
FILE COVERS 1968-1982


FILE SCISEARCH
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FILE COVERS 1974 TO 18 Jun 2009 (20090618/ED)

SCISEARCH has been reloaded, see HELP RLOAD for details.

FILE CONFSCI
FILE COVERS 1973 TO 30 Mar 2009 (20090330/ED)

CSA has resumed updates, see NEWS FILE

FILE DISSABS
FILE COVERS 1861 TO 28 MAY 2009 (20090528/ED)

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FILE COVERS 1960 TO DATE

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